identification.

```
L37             1 SEA FILE=CASREACT ABB=ON  "CLEUGH ERNEST STEPHEN"/AU


=> s l37 or (l37 and l31,l36)
L41             1 L37 OR (L37 AND (L31 OR L36))

=> dup rem l41,l40
FILE 'CASREACT' ENTERED AT 10:45:56 ON 18 DEC 2006
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FILE 'CAPLUS' ENTERED AT 10:45:56 ON 18 DEC 2006
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PROCESSING COMPLETED FOR L41
PROCESSING COMPLETED FOR L40
L42             2 DUP REM L41 L40 (1 DUPLICATE REMOVED)
                  ANSWER '1' FROM FILE CASREACT
                  ANSWER '2' FROM FILE CAPLUS

=> d ibib abs hit 1; d ibib ed abs hitstr 2


L42  ANSWER 1 OF 2  CASREACT  COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         142:463452  CASREACT  Full-text
TITLE:                    Production process of optically pure
                          2-(4-hydroxyphenoxy)propionic acid
INVENTOR(S):              Cleugh, Ernest Stephen
PATENT ASSIGNEE(S):       Syngenta Limited, UK
SOURCE:                   PCT Int. Appl., 10 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

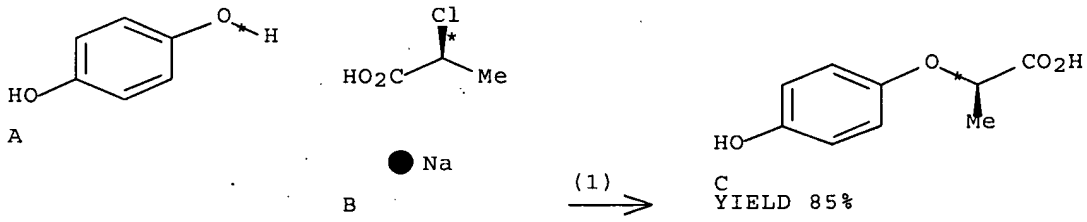
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2005042460      A1   20050512       WO 2004-GB3497   20040816
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
            SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
            SN, TD, TG
     CA 2535039         A1   20050512       CA 2004-2535039  20040816
     EP 1670743         A1   20060621       EP 2004-768060   20040816
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     CN 1852884         A    20061025       CN 2004-80026709 20040816
     BR 2004014925      A    20061107       BR 2004-14925    20040816
```

US 2006270851 A1 20061130 US 2006-571863 20060314
PRIORITY APPLN. INFO.: GB 2003-22917 20030930
WO 2004-GB3497 20040816

AB A process for producing optically pure (R)-2-(4-hydroxyphenoxy)propanoic acid (I) or a salt or ester thereof comprises reaction of hydroquinone or a salt thereof with a (S)-2-halopropanoic acid or a salt thereof in the presence of a mild reducing agent. This process prevents over-alkylation which gives bis(1-carboxyethoxy)benzene, and oxidation of hydroquinone which results in highly colored byproducts. The compound I is useful as an intermediate in making herbicidal products (e.g. quizalofop-P-Et and haloxyfop-P-methyl) in industrial scale. Thus, hydroquinone (574 g, 5.22 mol) was charged to a reaction flask followed by sodium bisulfite (5.74 g) and water (1,014 g). The mixture was stirred under N and heated to 50° and 47% sodium hydroxide solution (799.5 g, 9.39 mol) was added. The solution was heated to 65° and an aqueous solution of (S)-2-chloropropanoic acid sodium salt (544.4 g, 32.5% as the free acid, 1.63 mol) was added. The reaction mixture was held at 65° for 4 h to give the total reaction mass (2937.6 g) with I content of 8.60 %, equivalent to 252.5 g product or 85% yield. H2O (700 g) was added and the temperature adjusted to below 45°. H3PO4 (120 g) was added to adjust the pH to about 11 and then 98% sulfuric acid (250 g) was added to reduce the pH to 6,5-7.5, the temperature being controlled at 55° during these addns. The solution was then extracted with Me iso-Bu ketone to give a solution of hydroquinone in MiBK for use in the next cycle. The aqueous phase was then acidified to pH 2±0.2 using 98% H2SO4 and extracted with MiBK to give a solution of I which was washed with a solution of 155.5 g KOH and 2.15 g sodium bisulfite in 280 g H2O. The aqueous solution was acidified to pH 1 with 32% HCl, cooled to 20°, and filtered to give, after washing the solid with water, 62% I.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 1 A + B ===> C



RX(1) RCT A 123-31-9

STAGE(1)
RGT D 7631-90-5 NaHSO3
SOL 7732-18-5 Water
CON room temperature -> 50 deg C

STAGE(2)
RGT E 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 50 deg C -> 65 deg C

STAGE(3)

RCT B 74533-11-2
SOL 7732-18-5 Water
CON 4 hours, 65 deg C

STAGE(4)
RGT F 7732-18-5 Water
CON <45 deg C

STAGE(5)
RGT G 7664-38-2 H3PO4
SOL 7732-18-5 Water
CON 55 deg C, pH 11

STAGE(6)
RGT H 7664-93-9 H2SO4
SOL 7732-18-5 Water
CON 55 deg C, pH 6.5 - 7.5

STAGE(7)
RGT D 7631-90-5 NaHSO3, I 1310-58-3 KOH
SOL 7732-18-5 Water
CON room temperature

STAGE(8)
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON 20 deg C, pH 1

PRO C 94050-90-5
NTE stereoselective, workup, inert, industrial manufacture, hydroquinone can be recycled by extraction with methylisobutyl ketone

IN **Cleugh, Ernest Stephen**

L42 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:245553 CAPLUS Full-text
DOCUMENT NUMBER: 120:245553
TITLE: Isomerization process for pyrethroids
INVENTOR(S): **Cleugh, Ernest Stephen**; Milner, David John
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Brit. UK Pat. Appl., 11 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2262737	A	19930630	GB 1992-25856	19921211
WO 9313053	A2	19930708	WO 1992-GB2323	19921215
WO 9313053	A3	19930805		
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9230932	A	19930728	AU 1992-30932	19921215

AU 679168	B2	19970626			
EP 618896	A1	19941012	EP 1992-924842		19921215
EP 618896	B1	19960911			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
JP 07502995	T	19950330	JP 1993-511234		19921215
JP 3490083	B2	20040126			
BR 9206983	A	19951205	BR 1992-6983		19921215
HU 71704	A2	19960129	HU 1994-1811		19921215
HU 214673	B	19980428			
AT 142617	T	19960915	AT 1992-924842		19921215
ES 2091497	T3	19961101	ES 1992-924842		19921215
RO 114125	B1	19990129	RO 1994-1080		19921215
RU 2129536	C1	19990427	RU 1994-31154		19921215
CZ 287245	B6	20001011	CZ 1994-1536		19921215
SK 281750	B6	20010710	SK 1994-760		19921215
CA 2126180	C	20030506	CA 1992-2126180		19921215
ZA 9209971	A	19930707	ZA 1992-9971		19921222
US 5334744	A	19940802	US 1992-995861		19921223
FI 9402989	A	19940621	FI 1994-2989		19940621
FI 114465	B1	20041029			
NO 9402400	A	19940811	NO 1994-2400		19940623
NO 300678	B1	19970707			
PRIORITY APPLN. INFO.:			GB 1991-27355	A	19911224
			CS 1994-1536	A	19921215
			WO 1992-GB2323	A	19921215

OTHER SOURCE(S): MARPAT 120:245553

ED Entered STN: 14 May 1994

AB A process for obtaining an isomer of a compound of general formula RCH(CN)R' (I), (each of R and R' may be any organic radical linked directly or through a heteroatom to the carbon atom bearing the cyano group provided that at least one of R and R' comprises at least one resolved chiral center) which comprises the step of treating the epimer of the isomer, or the racemate comprising the epimer and the enantiomer of the epimer, in solution in a polar organic solvent, or in slurry in a polar organic liquid diluent in which the epimer or the racemate is partially soluble, with a source of cyanide ions, in the absence of a base, the isomer, or the racemic modification comprising the isomer and its enantiomer, being less soluble in the solvent or diluent than the epimer of the isomer, or the racemate comprising the epimer of the isomer and the enantiomer of the epimer, resp. The compound of formula I may be a pyrethroid, e.g. deltamethrin, acrinathrin, S-fenvalerate or λ-cyhalothrin.

CLAIM 1

=> fil capl; d que l24
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FILE COVERS 1907 - 18 Dec 2006 VOL 145 ISS 26
FILE LAST UPDATED: 17 Dec 2006 (20061217/ED)

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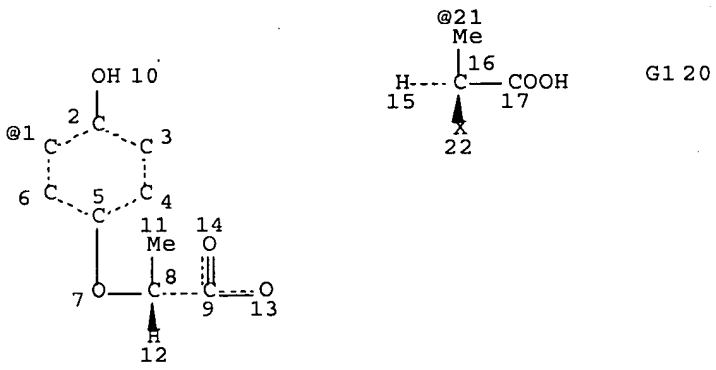
http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L17 STR



VAR G1=1/21
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 2
L19 72 SEA FILE=REGISTRY SSS FUL L17

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L20          49 SEA FILE=REGISTRY ABB=ON  46.150.18/RID AND L19
L21          23 SEA FILE=REGISTRY ABB=ON  L19 NOT L20
L22         412 SEA FILE=CAPLUS ABB=ON  L21
L23         115 SEA FILE=CAPLUS ABB=ON  L20
L24          15 SEA FILE=CAPLUS ABB=ON  L22 AND L23


=> s l24 not l40
L43          14 L24 NOT L40

=> fil casrea; d stat que l31
FILE 'CASREACT' ENTERED AT 10:47:13 ON 18 DEC 2006
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FILE CONTENT:1840 - 17 Dec 2006 VOL 145 ISS 25

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*************************************************************
*                                                           *
*     CASREACT now has more than 10 million reactions       *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.


L26             STR
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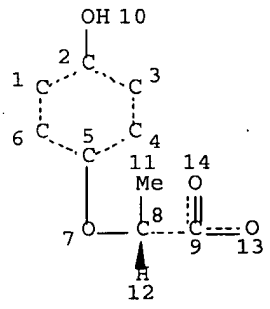


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14
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STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1
L28           97 SEA FILE=CASREACT SSS FUL L26 (    747 REACTIONS)
L29              STR
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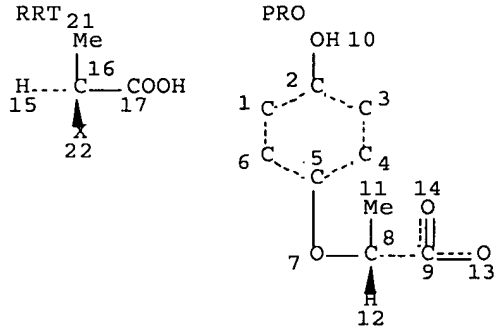

RRT=REACTANT OR REAGENT
PRO=PRODUCT

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  19

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 2
L31            5 SEA FILE=CASREACT SUB=L28 SSS FUL L29 (     18 REACTIONS)

100.0% DONE      28 VERIFIED      18 HIT RXNS                    5 DOCS
SEARCH TIME: 00.00.01



=> s l31 not l41
L44            4 L31 NOT L41

=> dup rem l44,l43
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PROCESSING COMPLETED FOR L44
PROCESSING COMPLETED FOR L43
L45           16 DUP REM L44 L43 (2 DUPLICATES REMOVED)
                 ANSWERS '1-4' FROM FILE CASREACT
                 ANSWERS '5-16' FROM FILE CAPLUS

=> d ibib abs hit 1-4; d ibib ed abs hitstr 5-16
```

L45 ANSWER 1 OF 16 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 113:40160 CASREACT Full-text
TITLE: Preparation and purification of D-[2-(4-hydroxyphenoxy)]propionic acid as a herbicide intermediate
INVENTOR(S): Moyne, Jose
PATENT ASSIGNEE(S): Rhone-Poulenc Chimie SA, Fr.
SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 352168	A1	19900124	EP 1989-401971	19890710
EP 352168	B1	19930616		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2634481	A1	19900126	FR 1988-9793	19880720
FR 2634481	B1	19900914		
JP 02048545	A	19900219	JP 1989-148515	19890613
JP 05033937	B	19930520		
AT 90658	T	19930715	AT 1989-401971	19890710
ES 2058571	T3	19941101	ES 1989-401971	19890710
DK 8903570	A	19900121	DK 1989-3570	19890719
CA 1323039	C	19931012	CA 1989-606124	19890719
US 4981998	A	19910101	US 1989-382312	19890720
PRIORITY APPLN. INFO.:			FR 1988-9793	19880720
			EP 1989-401971	19890710

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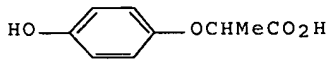
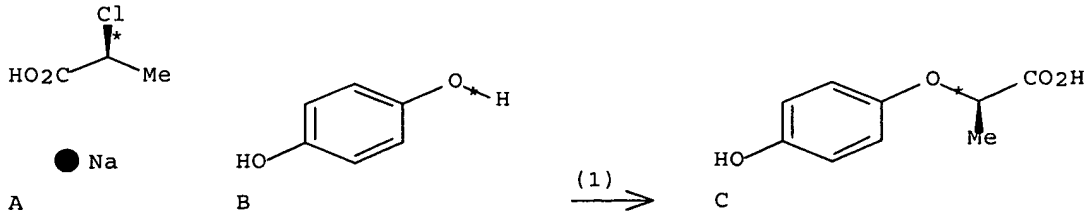


I

AB The title compound (I) was prepared and purified as follows. Reaction of MeCHClCO2Na (L-isomer) with p-NaOC6H4ONa, followed by adjustment of the reaction mixture to pH 1, removal of a part of the aqueous layer containing salts, addition of H2O, heating, and then cooling, gave optically pure I.

RX(1) OF 3 ...A + B ===> C



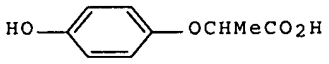
A B C

RX(1) RCT A 74533-11-2, B 123-31-9
PRO C 94050-90-5

L45 ANSWER 2 OF 16 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 106:18108 CASREACT Full-text
TITLE: Optically active 2-(4-hydroxyphenoxy)propionic acid
INVENTOR(S): Fujinawa, Shoji; Hashiba, Isao; Suzuki, Kenji; Tsuchiya, Shuji; Takakuwa, Yasuo
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61158947	A	19860718	JP 1984-279711	19841228
JP 06010154	B	19940209		
US 4625053	A	19861125	US 1985-794566	19851106
CA 1257874	A1	19890725	CA 1985-494991	19851112
EP 192849	A1	19860903	EP 1985-116097	19851217
EP 192849	B1	19880831		
R: CH, DE, FR, GB, IT, LI, NL				
PRIORITY APPLN. INFO.:			JP 1984-279711	19841228

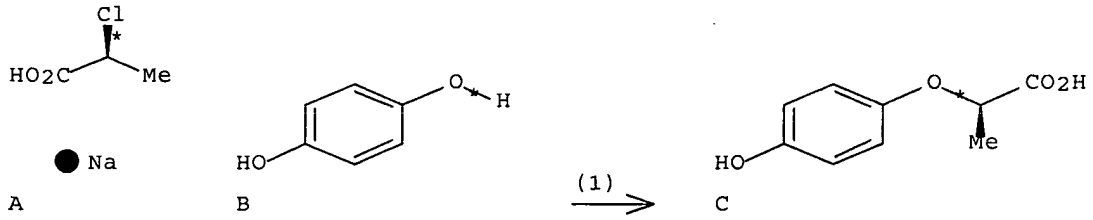
OTHER SOURCE(S): MARPAT 106:18108
GI



I

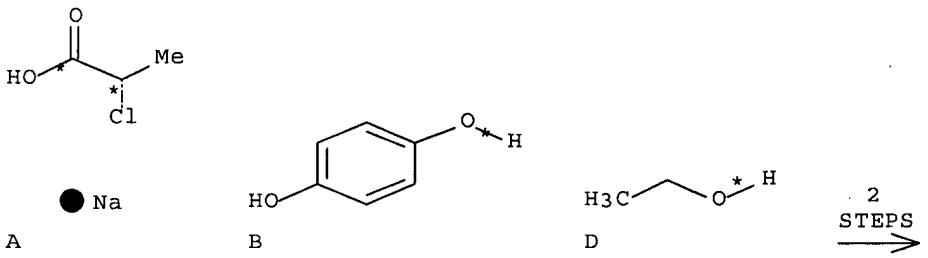
AB The title acid (I), useful as an intermediate for herbicides (no data), is prepared by reaction of XCHMeCO2M (II; X = Cl, Br; M = H, alkali metal) with hydroquinone (III) or its alkali salts in the presence of alkali hydroxides and H2O. Thus, saponification of 98 g 1-ClCHMeCO2Me with aqueous NaOH at 20-40° gave 1-II (X = Cl, M = Na), which was treated with 110 g II in H2O at 40° under N to give d-I, which was esterified with EtOH in the presence of H2SO4 to give 147 g d-I Et ester with 93% enantiomer excess.

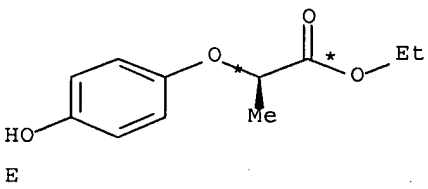
RX(1) OF 6 ...A + B ===> C...



RX(1) RCT A 74533-11-2, B 123-31-9
PRO C 94050-90-5

RX(4) OF 6 COMPOSED OF RX(1), RX(2)
RX(4) A + B + D ===> E





E

RX(1) RCT A 74533-11-2, B 123-31-9
PRO C 94050-90-5

RX(2) RCT C 94050-90-5, D 64-17-5
PRO E 71301-98-9

L45 ANSWER 3 OF 16 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 143:422130 CASREACT Full-text
TITLE: Process for the preparation of substituted tetralin and substituted indane derivatives
INVENTOR(S): Zhang-Plasket, Fan; Zhong, Hua; Villani, Frank
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 64 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005240049	A1	20051027	US 2005-110459	20050420
AU 2005238485	A1	20051110	AU 2005-238485	20050420
WO 2005105737	A1	20051110	WO 2005-US13870	20050420

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-564159P 20040421
WO 2005-US13870 20050420

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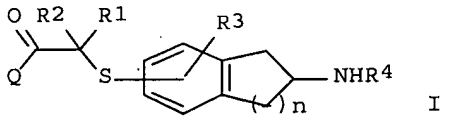
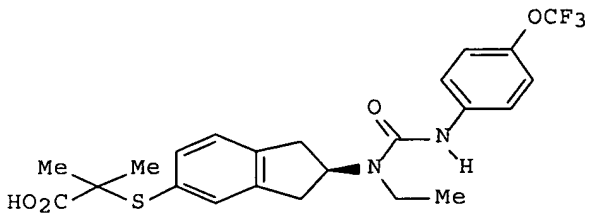


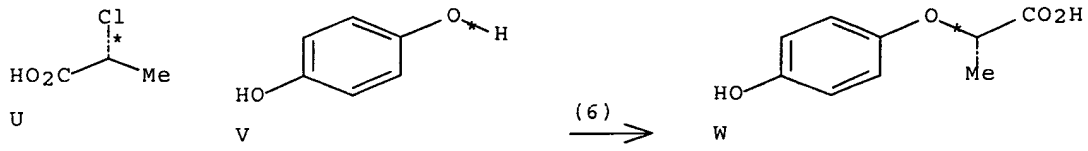
I



II

AB The present invention relates to novel processes for the preparation of substituted tetralin. and substituted indane derivs I [Q = OH, NH2, or O-protected or N-protected group; R1 and R2 independently = H, alkyl, alkoxyalkyl, etc.; R3 = H, alkoxy, halo, etc.; R4 = H, alkoxy, alkenyl, etc.; n = 1-6]. Thus, e.g., II was prepared via diastereomeric resolution of tert-Bu 2-(2-ethylaminoindan-5-ylsulfanyl)-2-methylpropionate (preparation given) followed by amidation with 4-(trifluoromethoxy)phenyl isocyanate and subsequent deprotection. The present invention is further directed to novel processes for the preparation of intermediates in the preparation of the substituted tetralin and substituted indane derivs.

RX(6) OF 145 U + V ===> W...



RX(6) RCT U **7474-05-7**

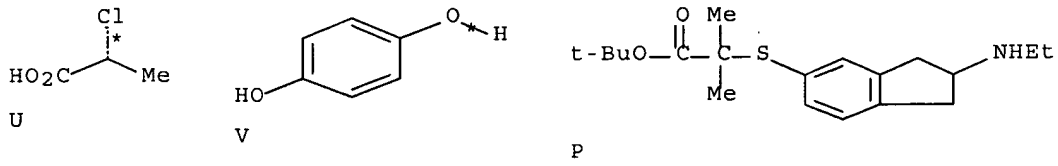
STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

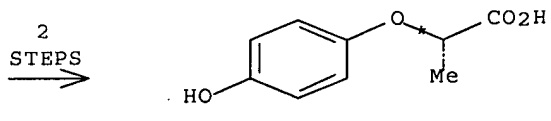
STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

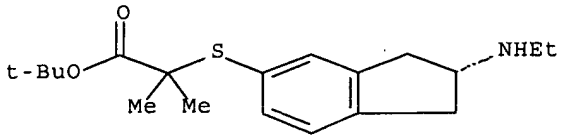
PRO W **105118-15-8**
NTE stereoselective

RX(37) OF 145 COMPOSED OF RX(6), RX(7)
RX(37) **U + V + P ===> X**





X: CM 1



X: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

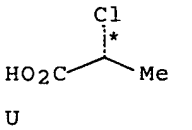
STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

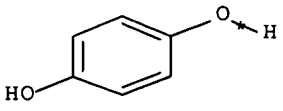
PRO W 105118-15-8
NTE stereoselective

RX(7) RCT P 685832-40-0, W 105118-15-8
PRO X 868159-07-3
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 30 - 35 deg C
SUBSTAGE(2) 2 hours, 0 deg C
NTE stereoselective

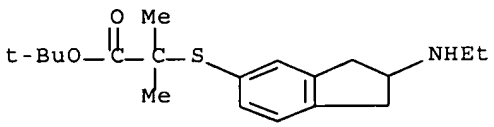
RX(38) OF 145 COMPOSED OF RX(6), RX(13)
RX(38) **U + V + P ===> AJ**



U

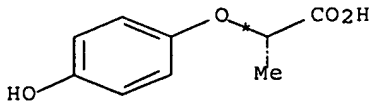


V

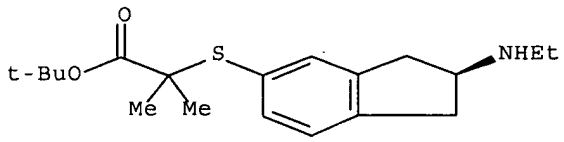


P

2 STEPS



AJ: CM 1



AJ: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

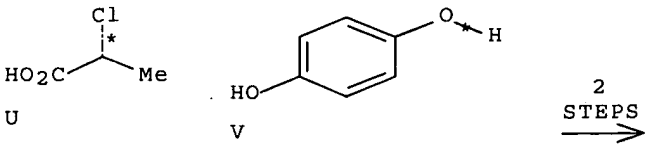
STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

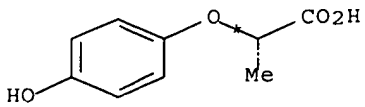
PRO W 105118-15-8
NTE stereoselective

RX(13) RCT P 685832-40-0, W 105118-15-8
PRO AJ 868159-12-0
SOL 109-99-9 THF
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) overnight, room temperature
NTE stereoselective

RX(60) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(7)
AND REACTION SEQUENCE RX(5), RX(7)
... U + V ===> W...
...M + O + W ===> X

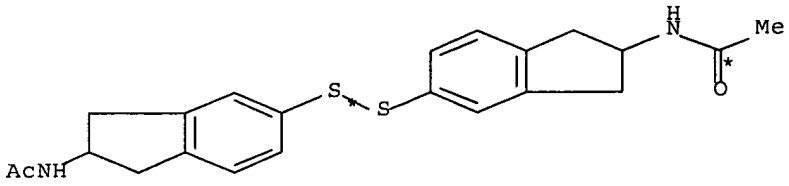


U V 2 STEPS

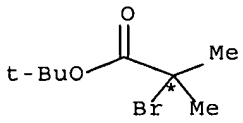


W

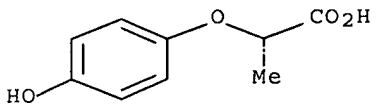
START NEXT REACTION SEQUENCE



M

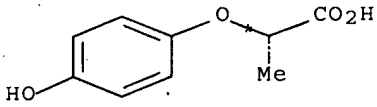


O

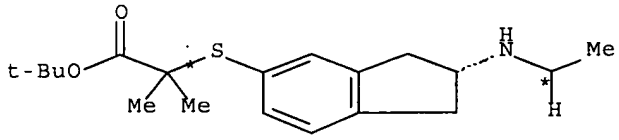


W

2 STEPS



X: CM 1



X: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

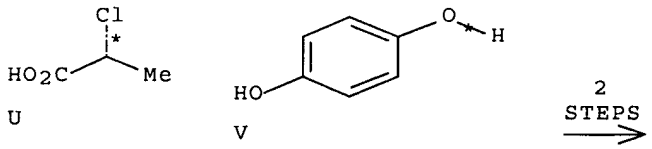
STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

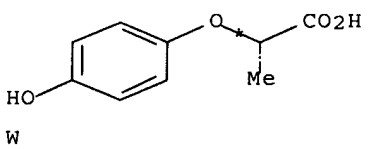
STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

PRO P 685832-40-0

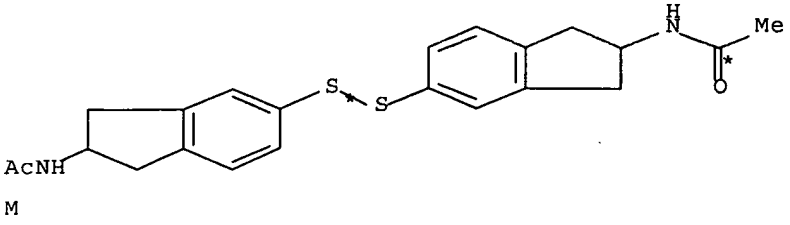
RX(7) RCT P 685832-40-0, W 105118-15-8
PRO X 868159-07-3
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 30 - 35 deg C
SUBSTAGE(2) 2 hours, 0 deg C
NTE stereoselective

RX(61) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(13)
AND REACTION SEQUENCE RX(5), RX(13)
... U + V ===> W...
...M + O + W ===> AJ

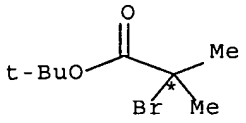




START NEXT REACTION SEQUENCE



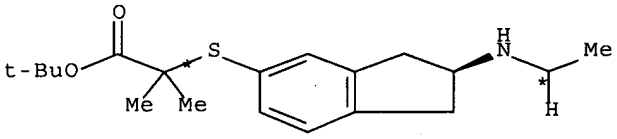
M



O

W

AJ: CM 1



AJ: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4

SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

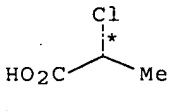
STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

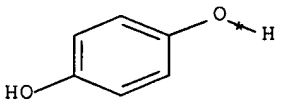
PRO P 685832-40-0

RX(13) RCT P 685832-40-0, W 105118-15-8
PRO AJ 868159-12-0
SOL 109-99-9 THF
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) overnight, room temperature
NTE stereoselective

RX(63) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(7)
AND REACTION SEQUENCE RX(4), RX(5), RX(7)
... U + V ===> W...
...2 J + O + W ===> X

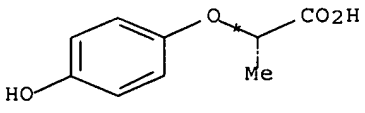


U



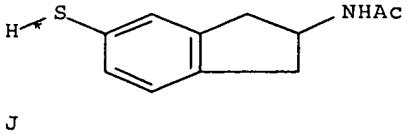
V

3
STEPS

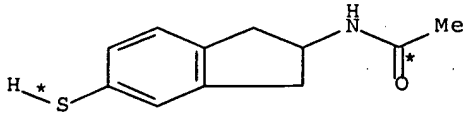


W

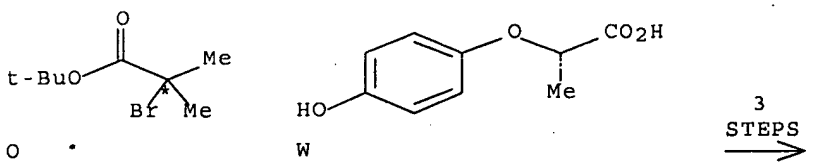
START NEXT REACTION SEQUENCE



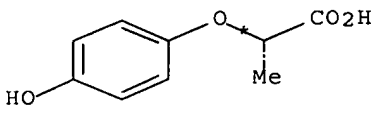
J



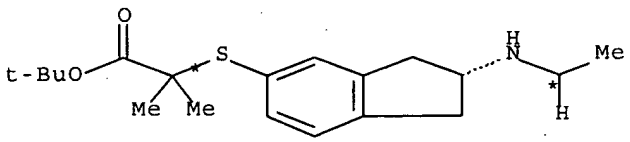
J



O W



X: CM 1



X: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(4) RCT J 74124-94-0

STAGE(1)
RGT K 7440-66-6 Zn
SOL 75-05-8 MeCN
CON room temperature

STAGE(2)
RGT N 75-78-5 Me2SiCl2
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
SUBSTAGE(2) 20 hours, room temperature

PRO M 868159-05-1

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

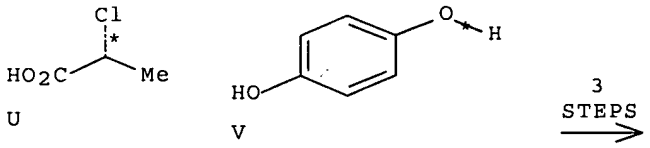
STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

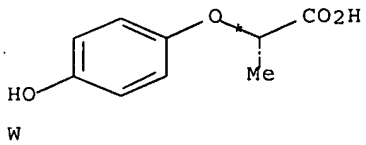
STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

PRO P 685832-40-0

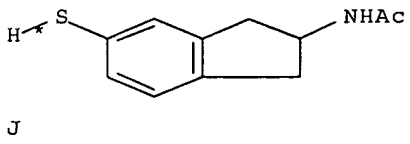
RX(7) RCT P 685832-40-0, W 105118-15-8
PRO X 868159-07-3
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 30 - 35 deg C
SUBSTAGE(2) 2 hours, 0 deg C
NTE stereoselective

RX(64) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(13)
AND REACTION SEQUENCE RX(4), RX(5), RX(13)
... U + V ===> W...
...2 J + O + W ===> AJ

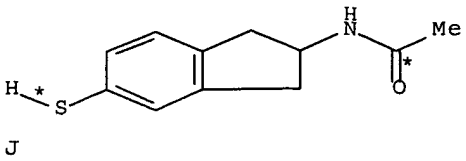




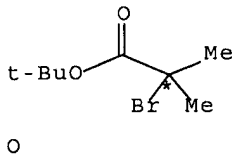
START NEXT REACTION SEQUENCE



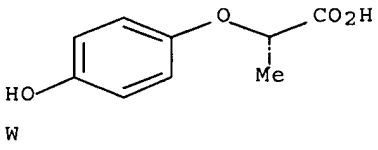
J



J

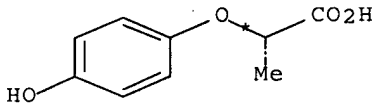


O

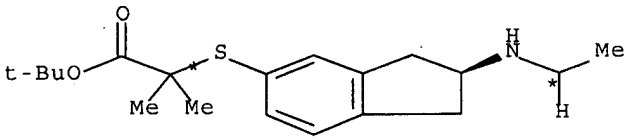


W

3 STEPS



AJ: CM 1



AJ: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(4) RCT J 74124-94-0

STAGE(1)
RGT K 7440-66-6 Zn
SOL 75-05-8 MeCN
CON room temperature

STAGE(2)

RGT N 75-78-5 Me2SiCl2
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
SUBSTAGE(2) 20 hours, room temperature

PRO M 868159-05-1

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

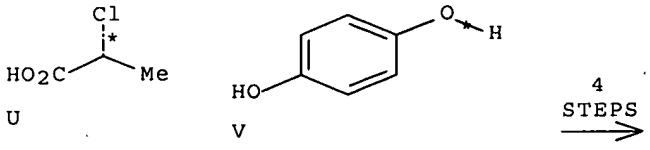
STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

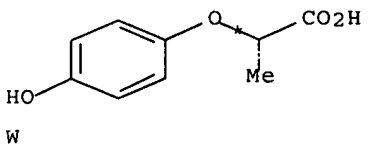
STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

PRO P 685832-40-0

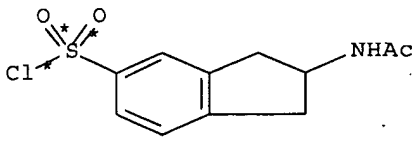
RX(13) RCT P 685832-40-0, W 105118-15-8
PRO AJ 868159-12-0
SOL 109-99-9 THF
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) overnight, room temperature
NTE stereoselective

RX(90) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(7)
AND REACTION SEQUENCE RX(3), RX(4), RX(5), RX(7)
... U + V ===> W...
...2 G + O + W ===> X





START NEXT REACTION SEQUENCE



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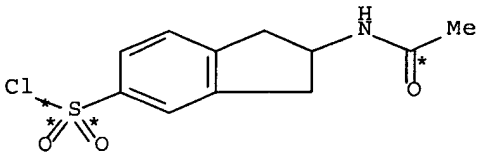

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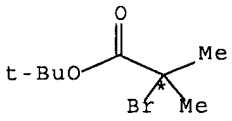

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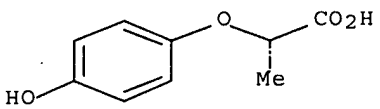
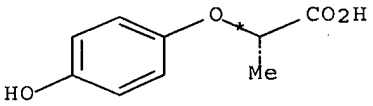
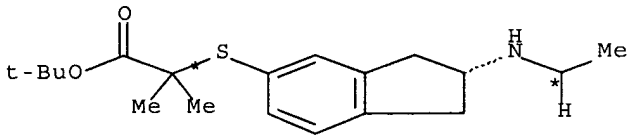


W

4
STEPS



X: CM 1



X: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(3) RCT G 74124-92-8

```
            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  50 - 60 deg C

            STAGE(2)
               RGT  L 7647-01-0 HCl
               SOL  7732-18-5 Water
               CON  SUBSTAGE(1) 1 hour, 70 - 75 deg C
                    SUBSTAGE(2) 30 minutes, 75 deg C -> 30 deg C

         PRO  J 74124-94-0

RX(4)    RCT  J 74124-94-0

            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  room temperature

            STAGE(2)
               RGT  N 75-78-5 Me2SiCl2
               SOL  75-05-8 MeCN
               CON  SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
                    SUBSTAGE(2) 20 hours, room temperature

         PRO  M 868159-05-1

RX(5)    RCT  M 868159-05-1

            STAGE(1)
               RGT  Q 16853-85-3 LiAlH4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) 25 minutes, 60 - 66 deg C
                    SUBSTAGE(2) 4 hours, reflux

            STAGE(2)
               RGT  R 67-56-1 MeOH
               CON  <25 deg C

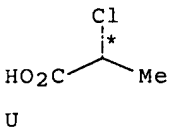
            STAGE(3)
               RCT  O 23877-12-5
               CON  SUBSTAGE(1) 5 - 7 deg C
                    SUBSTAGE(2) 2 hours, room temperature

            STAGE(4)
               RGT  S 1310-73-2 NaOH
               SOL  7732-18-5 Water
               CON  room temperature

         PRO  P 685832-40-0

RX(7)    RCT  P 685832-40-0, W 105118-15-8
         PRO  X 868159-07-3
         SOL  7732-18-5 Water, 64-17-5 EtOH
         CON  SUBSTAGE(1) 30 - 35 deg C
              SUBSTAGE(2) 2 hours, 0 deg C
         NTE  stereoselective
```

RX(91) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(13)
AND REACTION SEQUENCE RX(3), RX(4), RX(5), RX(13)
... U + V ===> W...
...2 G + O + W ===> **AJ**



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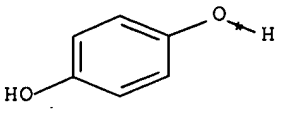
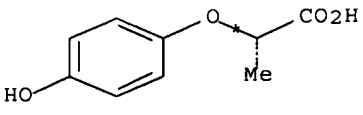


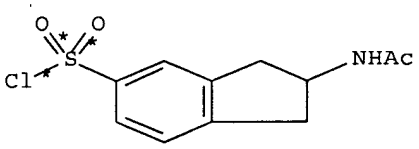
V

4
STEPS



W

START NEXT REACTION SEQUENCE



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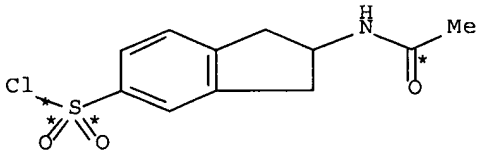

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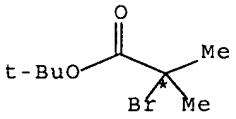

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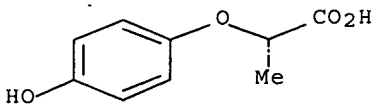
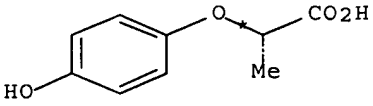
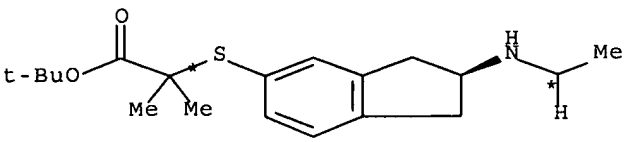


W

4
STEPS



AJ: CM 1



AJ: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)

```
            RGT  S 1310-73-2 NaOH
            SOL  7732-18-5 Water
            CON  <25 deg C

          STAGE(2)
            RCT  V 123-31-9
            RGT  S 1310-73-2 NaOH
            SOL  7732-18-5 Water
            CON  SUBSTAGE(1) <55 deg C
                 SUBSTAGE(2) 2 hours, 55 - 60 deg C

          STAGE(3)
            RGT  L 7647-01-0 HCl
            SOL  7732-18-5 Water
            CON  15 - 30 deg C, pH 4.3

        PRO  W 105118-15-8
        NTE  stereoselective

RX(3)   RCT  G 74124-92-8

          STAGE(1)
            RGT  K 7440-66-6 Zn
            SOL  75-05-8 MeCN
            CON  50 - 60 deg C

          STAGE(2)
            RGT  L 7647-01-0 HCl
            SOL  7732-18-5 Water
            CON  SUBSTAGE(1) 1 hour, 70 - 75 deg C
                 SUBSTAGE(2) 30 minutes, 75 deg C -> 30 deg C

        PRO  J 74124-94-0

RX(4)   RCT  J 74124-94-0

          STAGE(1)
            RGT  K 7440-66-6 Zn
            SOL  75-05-8 MeCN
            CON  room temperature

          STAGE(2)
            RGT  N 75-78-5 Me2SiCl2
            SOL  75-05-8 MeCN
            CON  SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
                 SUBSTAGE(2) 20 hours, room temperature

        PRO  M 868159-05-1

RX(5)   RCT  M 868159-05-1

          STAGE(1)
            RGT  Q 16853-85-3 LiAlH4
            SOL  109-99-9 THF
            CON  SUBSTAGE(1) 25 minutes, 60 - 66 deg C
                 SUBSTAGE(2) 4 hours, reflux

          STAGE(2)
            RGT  R 67-56-1 MeOH
            CON  <25 deg C
```

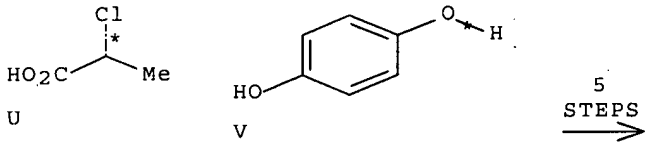
STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

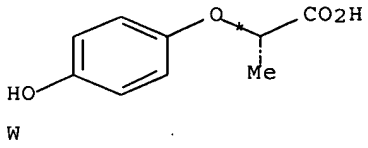
STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

PRO P 685832-40-0

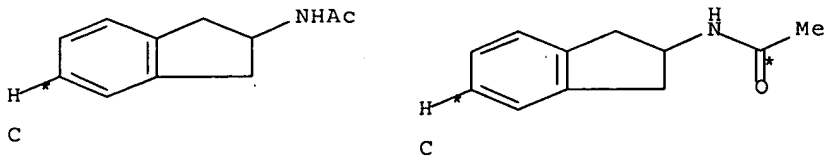
RX(13) RCT P 685832-40-0, W 105118-15-8
PRO AJ 868159-12-0
SOL 109-99-9 THF
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) overnight, room temperature
NTE stereoselective

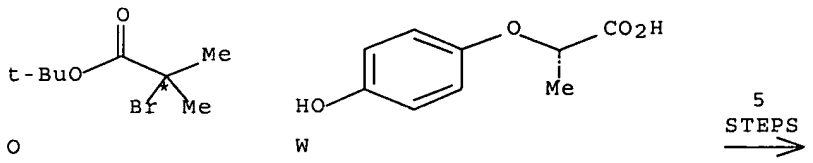
RX(93) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(7)
AND REACTION SEQUENCE RX(2), RX(3), RX(4), RX(5), RX(7)
... U + V ===> W...
...2 C + O + W ===> X





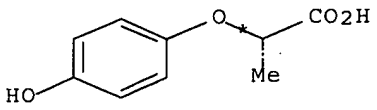
START NEXT REACTION SEQUENCE



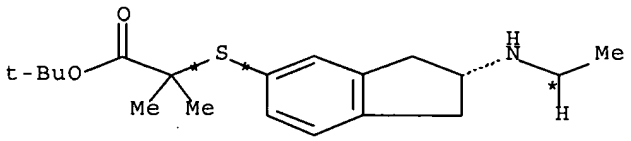


O W

5 STEPS



X: CM 1



X: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(2) RCT C 13935-80-3

STAGE(1)
SOL 75-05-8 MeCN
CON 3 - 5 deg C

STAGE(2)
RGT H 7790-94-5 ClSO3H
CON SUBSTAGE(1) 30 minutes, <15 deg C
SUBSTAGE(2) <15 deg C -> room temperature
SUBSTAGE(3) 30 minutes, room temperature -> 80 deg C
SUBSTAGE(4) 20 hours, 50 deg C

STAGE(3)
RGT E 7732-18-5 Water, I 75-05-8 MeCN
CON SUBSTAGE(1) 10 - 15 minutes, 5 deg C -> -6 deg C
SUBSTAGE(2) 30 minutes, 0 - 5 deg C

```
          PRO  G 74124-92-8

RX(3)     RCT  G 74124-92-8

            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  50 - 60 deg C

            STAGE(2)
               RGT  L 7647-01-0 HCl
               SOL  7732-18-5 Water
               CON  SUBSTAGE(1) 1 hour, 70 - 75 deg C
                    SUBSTAGE(2) 30 minutes, 75 deg C -> 30 deg C

          PRO  J 74124-94-0

RX(4)     RCT  J 74124-94-0

            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  room temperature

            STAGE(2)
               RGT  N 75-78-5 Me2SiCl2
               SOL  75-05-8 MeCN
               CON  SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
                    SUBSTAGE(2) 20 hours, room temperature

          PRO  M 868159-05-1

RX(5)     RCT  M 868159-05-1

            STAGE(1)
               RGT  Q 16853-85-3 LiAlH4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) 25 minutes, 60 - 66 deg C
                    SUBSTAGE(2) 4 hours, reflux

            STAGE(2)
               RGT  R 67-56-1 MeOH
               CON  <25 deg C

            STAGE(3)
               RCT  O 23877-12-5
               CON  SUBSTAGE(1) 5 - 7 deg C
                    SUBSTAGE(2) 2 hours, room temperature

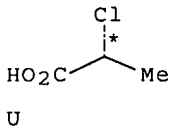
            STAGE(4)
               RGT  S 1310-73-2 NaOH
               SOL  7732-18-5 Water
               CON  room temperature

          PRO  P 685832-40-0

RX(7)     RCT  P 685832-40-0, W 105118-15-8
          PRO  X 868159-07-3
          SOL  7732-18-5 Water, 64-17-5 EtOH
```

CON SUBSTAGE(1) 30 - 35 deg C
SUBSTAGE(2) 2 hours, 0 deg C
NTE stereoselective

RX(94) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(13)
AND REACTION SEQUENCE RX(2), RX(3), RX(4), RX(5), RX(13)
... U + V ===> W...
...2 C + O + W ===> **AJ**



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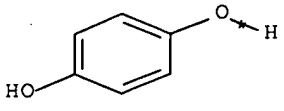
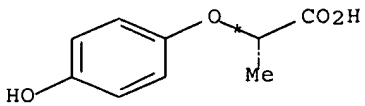


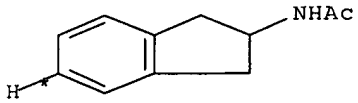
V

5 STEPS →

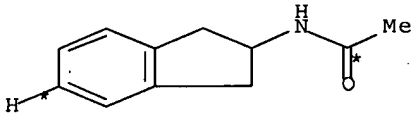


W

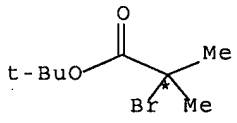
START NEXT REACTION SEQUENCE



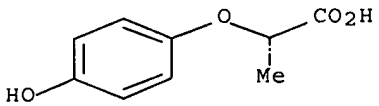
C



C

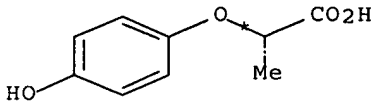


O

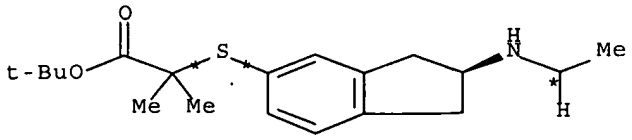


W

5 STEPS →



AJ: CM 1



AJ: CM 2

```
RX(6)     RCT  U 7474-05-7

            STAGE(1)
               RGT  S 1310-73-2 NaOH
               SOL  7732-18-5 Water
               CON  <25 deg C

            STAGE(2)
               RCT  V 123-31-9
               RGT  S 1310-73-2 NaOH
               SOL  7732-18-5 Water
               CON  SUBSTAGE(1) <55 deg C
                    SUBSTAGE(2) 2 hours, 55 - 60 deg C

            STAGE(3)
               RGT  L 7647-01-0 HCl
               SOL  7732-18-5 Water
               CON  15 - 30 deg C, pH 4.3

          PRO  W 105118-15-8
          NTE  stereoselective

RX(2)     RCT  C 13935-80-3

            STAGE(1)
               SOL  75-05-8 MeCN
               CON  3 - 5 deg C

            STAGE(2)
               RGT  H 7790-94-5 ClSO3H
               CON  SUBSTAGE(1) 30 minutes, <15 deg C
                    SUBSTAGE(2) <15 deg C -> room temperature
                    SUBSTAGE(3) 30 minutes, room temperature -> 80 deg C
                    SUBSTAGE(4) 20 hours, 50 deg C

            STAGE(3)
               RGT  E 7732-18-5 Water, I 75-05-8 MeCN
               CON  SUBSTAGE(1) 10 - 15 minutes, 5 deg C -> -6 deg C
                    SUBSTAGE(2) 30 minutes, 0 - 5 deg C

          PRO  G 74124-92-8

RX(3)     RCT  G 74124-92-8

            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  50 - 60 deg C

            STAGE(2)
               RGT  L 7647-01-0 HCl
               SOL  7732-18-5 Water
               CON  SUBSTAGE(1) 1 hour, 70 - 75 deg C
                    SUBSTAGE(2) 30 minutes, 75 deg C -> 30 deg C

          PRO  J 74124-94-0

RX(4)     RCT  J 74124-94-0

            STAGE(1)
```

RGT K 7440-66-6 Zn
SOL 75-05-8 MeCN
CON room temperature

STAGE(2)
RGT N 75-78-5 Me2SiCl2
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
SUBSTAGE(2) 20 hours, room temperature

PRO M 868159-05-1

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

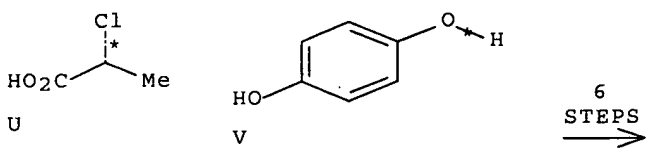
STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

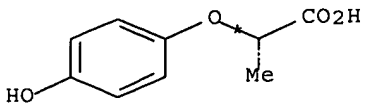
PRO P 685832-40-0

RX(13) RCT P 685832-40-0, W 105118-15-8
PRO AJ 868159-12-0
SOL 109-99-9 THF
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) overnight, room temperature
NTE stereoselective

RX(96) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(7)
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(5), RX(7)

... U + V ===> W...
...2 A + 2 B + O + W ===> X





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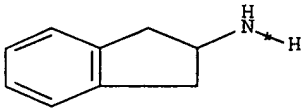
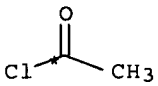
START NEXT REACTION SEQUENCE



2 A



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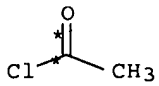

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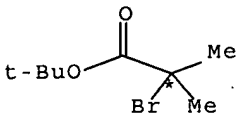

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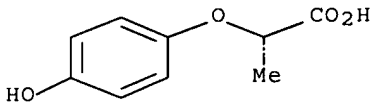
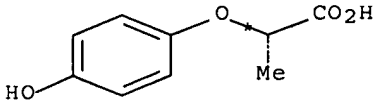
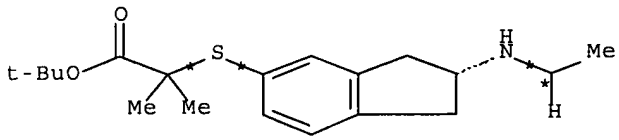


W

6 STEPS



X: CM 1



X: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

```
          PRO  W 105118-15-8
          NTE  stereoselective

RX(1)     RCT  A 2975-41-9

            STAGE(1)
               RGT  D 497-19-8 Na2CO3
               SOL  7732-18-5 Water, 141-78-6 AcOEt
               CON  5 - 7 deg C

            STAGE(2)
               RCT  B 75-36-5
               CON  SUBSTAGE(1) 2 hours, <10 deg C
                    SUBSTAGE(2) 1 hour, room temperature

          PRO  C 13935-80-3

RX(2)     RCT  C 13935-80-3

            STAGE(1)
               SOL  75-05-8 MeCN
               CON  3 - 5 deg C

            STAGE(2)
               RGT  H 7790-94-5 ClSO3H
               CON  SUBSTAGE(1) 30 minutes, <15 deg C
                    SUBSTAGE(2) <15 deg C -> room temperature
                    SUBSTAGE(3) 30 minutes, room temperature -> 80 deg C
                    SUBSTAGE(4) 20 hours, 50 deg C

            STAGE(3)
               RGT  E 7732-18-5 Water, I 75-05-8 MeCN
               CON  SUBSTAGE(1) 10 - 15 minutes, 5 deg C -> -6 deg C
                    SUBSTAGE(2) 30 minutes, 0 - 5 deg C

          PRO  G 74124-92-8

RX(3)     RCT  G 74124-92-8

            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  50 - 60 deg C

            STAGE(2)
               RGT  L 7647-01-0 HCl
               SOL  7732-18-5 Water
               CON  SUBSTAGE(1) 1 hour, 70 - 75 deg C
                    SUBSTAGE(2) 30 minutes, 75 deg C -> 30 deg C

          PRO  J 74124-94-0

RX(4)     RCT  J 74124-94-0

            STAGE(1)
               RGT  K 7440-66-6 Zn
               SOL  75-05-8 MeCN
               CON  room temperature

            STAGE(2)
```

RGT N 75-78-5 Me2SiCl2
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
SUBSTAGE(2) 20 hours, room temperature

PRO M 868159-05-1

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

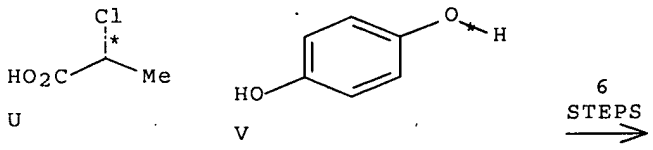
STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

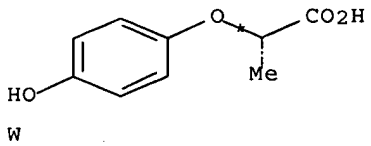
STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

PRO P 685832-40-0

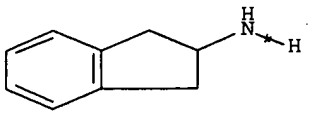
RX(7) RCT P 685832-40-0, W 105118-15-8
PRO X 868159-07-3
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 30 - 35 deg C
SUBSTAGE(2) 2 hours, 0 deg C
NTE stereoselective

RX(97) OF 145 COMPOSED OF REACTION SEQUENCE RX(6), RX(13)
AND REACTION SEQUENCE RX(1), RX(2), RX(3), RX(4), RX(5), RX(13)
... U + V ===> W...
...2 A + 2 B + O + W ===> AJ

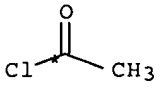




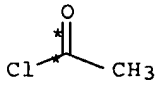
START NEXT REACTION SEQUENCE



2 A



B



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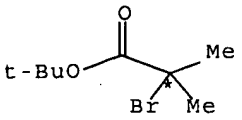

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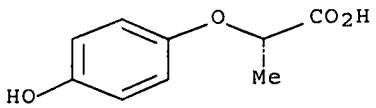
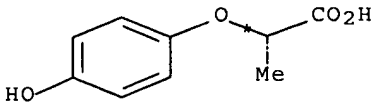
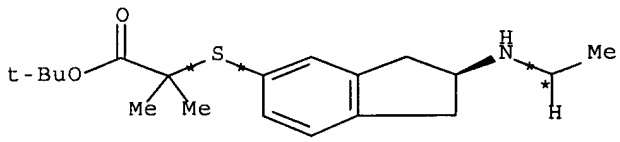


W

6 STEPS



AJ: CM 1



AJ: CM 2

RX(6) RCT U 7474-05-7

STAGE(1)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON <25 deg C

STAGE(2)
RCT V 123-31-9
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON SUBSTAGE(1) <55 deg C
SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(3)
RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON 15 - 30 deg C, pH 4.3

PRO W 105118-15-8
NTE stereoselective

RX(1) RCT A 2975-41-9

STAGE(1)
RGT D 497-19-8 Na2CO3

```
            SOL  7732-18-5 Water, 141-78-6 AcOEt
            CON  5 - 7 deg C

          STAGE(2)
            RCT  B 75-36-5
            CON  SUBSTAGE(1) 2 hours, <10 deg C
                 SUBSTAGE(2) 1 hour, room temperature

       PRO  C 13935-80-3

RX(2)  RCT  C 13935-80-3

          STAGE(1)
            SOL  75-05-8 MeCN
            CON  3 - 5 deg C

          STAGE(2)
            RGT  H 7790-94-5 ClSO3H
            CON  SUBSTAGE(1) 30 minutes, <15 deg C
                 SUBSTAGE(2) <15 deg C -> room temperature
                 SUBSTAGE(3) 30 minutes, room temperature -> 80 deg C
                 SUBSTAGE(4) 20 hours, 50 deg C

          STAGE(3)
            RGT  E 7732-18-5 Water, I 75-05-8 MeCN
            CON  SUBSTAGE(1) 10 - 15 minutes, 5 deg C -> -6 deg C
                 SUBSTAGE(2) 30 minutes, 0 - 5 deg C

       PRO  G 74124-92-8

RX(3)  RCT  G 74124-92-8

          STAGE(1)
            RGT  K 7440-66-6 Zn
            SOL  75-05-8 MeCN
            CON  50 - 60 deg C

          STAGE(2)
            RGT  L 7647-01-0 HCl
            SOL  7732-18-5 Water
            CON  SUBSTAGE(1) 1 hour, 70 - 75 deg C
                 SUBSTAGE(2) 30 minutes, 75 deg C -> 30 deg C

       PRO  J 74124-94-0

RX(4)  RCT  J 74124-94-0

          STAGE(1)
            RGT  K 7440-66-6 Zn
            SOL  75-05-8 MeCN
            CON  room temperature

          STAGE(2)
            RGT  N 75-78-5 Me2SiCl2
            SOL  75-05-8 MeCN
            CON  SUBSTAGE(1) 1 hour, room temperature -> 60 deg C
                 SUBSTAGE(2) 20 hours, room temperature

       PRO  M 868159-05-1
```

RX(5) RCT M 868159-05-1

STAGE(1)
RGT Q 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON SUBSTAGE(1) 25 minutes, 60 - 66 deg C
SUBSTAGE(2) 4 hours, reflux

STAGE(2)
RGT R 67-56-1 MeOH
CON <25 deg C

STAGE(3)
RCT O 23877-12-5
CON SUBSTAGE(1) 5 - 7 deg C
SUBSTAGE(2) 2 hours, room temperature

STAGE(4)
RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature

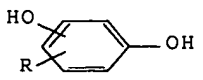
PRO P 685832-40-0

RX(13) RCT P 685832-40-0, W 105118-15-8
PRO AJ 868159-12-0
SOL 109-99-9 THF
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) overnight, room temperature
NTE stereoselective

L45 ANSWER 4 OF 16 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 95:150172 CASREACT Full-text
TITLE: Substituted phenoxycarboxylic acids
PATENT ASSIGNEE(S): Ihara Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56059718	A	19810523	JP 1979-135010	19791019

PRIORITY APPLN. INFO.: JP 1979-135010 19791019
GI



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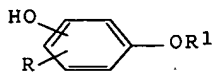
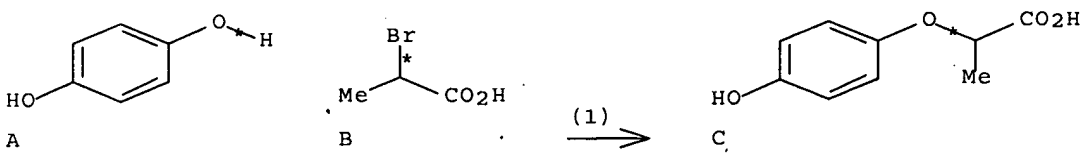


II

AB Phenols I (R = H, halo, nitro, cyano, alkyl, CF3) were treated with R1X (R1 = CHR2CO2R3, CH2CR2:CHCO2R3, etc., R2, R3 = H, alkyl), a base and a phase-

transfer catalyst to give II. Thus, heating hydroquinone with BrCHMeCO2H, K2CO3 and PhCH2NEt3Cl in H2O 3 h at 90° gave 65.5% 4-HOC6H4OCHMeCO2H.

RX(1) OF 1 A + B ===> C



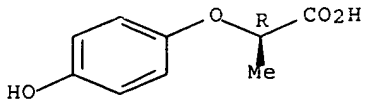
RX(1) RCT A 123-31-9, B 598-72-1
PRO C 67648-61-7

L45 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:995754 CAPLUS Full-text
DOCUMENT NUMBER: 124:116868
TITLE: Preparation of optically active α-(hydroxyphenoxy)alkanoates
INVENTOR(S): Metivier, M. Pascal
PATENT ASSIGNEE(S): Rhone-Poulenc Chimie SA, Fr.
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 679629	A1	19951102	EP 1995-400892	19950421
EP 679629	B1	19980812		
R: CH, DE, FR, GB, IT, LI				
FR 2719042	A1	19951027	FR 1994-4933	19940425
FR 2719042	B1	19960515		
JP 07291895	A	19951107	JP 1995-100907	19950425
US 5654338	A	19970805	US 1995-428710	19950425

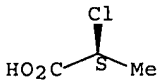
PRIORITY APPLN. INFO.: FR 1994-4933 A 19940425
OTHER SOURCE(S): CASREACT 124:116868; MARPAT 124:116868
ED Entered STN: 22 Dec 1995
AB The title process comprises saponification of an optically active α-haloester followed by condensation of the product with a hydroxyphenol. Thus, L-MeCHClCO2Me (97% optical purity) was converted in 75.3% yield to D-4-(HO)C6H4OCHMeCO2H of 96% optical purity.
IT **94050-90-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active α-(hydroxyphenoxy)alkanoates)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 29617-66-1, L-α-Chloropropionic acid methyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active α-(hydroxyphenoxy)alkanoates)
RN 29617-66-1 CAPLUS
CN Propanoic acid, 2-chloro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

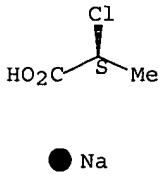


L45 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:168822 CAPLUS Full-text
DOCUMENT NUMBER: 118:168822
TITLE: Preparation of 2-(4-hydroxyphenoxy)propionic acid dicyclohexylamine salt
INVENTOR(S): Hashimoto, Masaki; Fukami, Jiichi
PATENT ASSIGNEE(S): Suntory, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04297438	A	19921021	JP 1991-63195	19910327

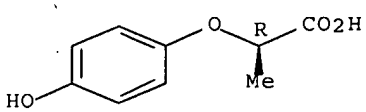
PRIORITY APPLN. INFO.: JP 1991-63195 19910327
OTHER SOURCE(S): CASREACT 118:168822
ED Entered STN: 01 May 1993
AB The title compound (I), useful as intermediate for herbicides, is prepared by treatment of reaction mixts. containing I and hydroquinone with dicyclohexylamine, followed by separation of the crystals. Hydroquinone (11 g) was treated with Na (RS)-2-chloropropionate in aqueous NaOH at 80° for 1 h, adjusted to pH 8, filtered to remove hydroquinone, and the filtrate was adjusted to pH 0.8, extracted with AcOEt, and treated with dicyclohexylamine to give 17 g (RS)-I.
IT 74533-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of, with hydroquinone)
RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 94050-90-5P, (R)-2-(4-Hydroxyphenoxy)propionic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and salt formation of, with dicyclohexylamine)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

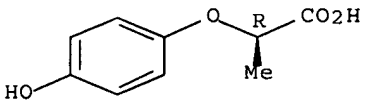


IT 146671-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for herbicides)
RN 146671-28-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (R)-, compd. with
N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

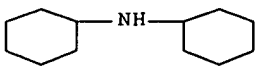
CRN 94050-90-5
CMF C9 H10 O4

Absolute stereochemistry. Rotation (+).



CM 2

CRN 101-83-7
CMF C12 H23 N



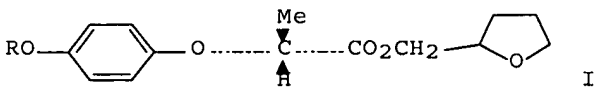
L45 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:449380 CAPLUS Full-text
DOCUMENT NUMBER: 115:49380
TITLE: Preparation of tetrahydrofurfuryl phenoxypropionates as herbicides or intermediates therefor
INVENTOR(S): Kagawa, Takumi; Ito, Mikio; Aman, Shunji; Morooka, Takashi; Watanabe, Eiroyuki; Tsuzuki, Kenji
PATENT ASSIGNEE(S): Tosoh Corp., Japan
SOURCE: Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 410758	A2	19910130	EP 1990-308209	19900726
EP 410758	A3	19921119		
R: BE, CH, DE, FR, GB, LI, NL				
JP 03056483	A	19910312	JP 1989-191252	19890726
JP 03204869	A	19910906	JP 1989-232861	19890911
JP 03106868	A	19910507	JP 1989-240266	19890918
JP 03127786	A	19910530	JP 1989-264984	19891013
JP 03145465	A	19910620	JP 1989-281805	19891031
JP 03157370	A	19910705	JP 1989-294805	19891115
JP 03184977	A	19910812	JP 1989-322574	19891214
US 5258521	A	19931102	US 1990-556716	19900725

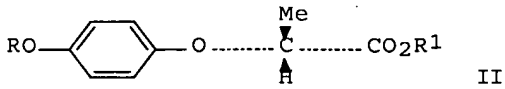
PRIORITY APPLN. INFO.:

JP 1989-191252	A	19890726
JP 1989-232861	A	19890911
JP 1989-240266	A	19890918
JP 1989-264984	A	19891013
JP 1989-281805	A	19891031
JP 1989-294805	A	19891115
JP 1989-322574	A	19891214

OTHER SOURCE(S): MARPAT 115:49380
ED Entered STN: 10 Aug 1991
GI



I



II

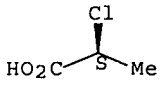
AB The title compds. I (R = H, 3-chloro-5-trifluoromethyl-2-pyridyl) were prepared by, e.g., (1) transesterification of ester II (R1 = Me) with tetrahydrofurfuryl alc. (III) in the presence of an acid catalyst; or (2) esterification of carboxylic acid II (R1 = H) with tetrahydrofurfuryl alc. in the presence of a hydrogen halide. Thus, II (R = 3-chloro-5- trifluoromethyl-

2-pyridyl; R1 = Me), III, and p-toluenesulfonic acid in benzene was refluxed for 5 h to give I (R = 3-chloro-5-trifluoromethyl-2- pyridyl).

IT **29617-66-1 94050-90-5 96562-58-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of herbicide intermediate)

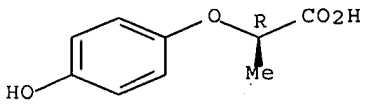
RN 29617-66-1 CAPLUS
CN Propanoic acid, 2-chloro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



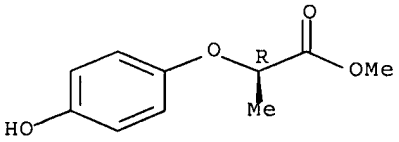
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 96562-58-2 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L45 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:608792 CAPLUS Full-text
DOCUMENT NUMBER: 115:208792
TITLE: Chiral liquid-crystalline polymers by polymer-analogous reactions
AUTHOR(S): Kapitza, Heinrich; Zentel, Rudolf
CORPORATE SOURCE: Inst. Org. Chem. Makromol. Chem., Heinrich-Heine-Univ., Duesseldorf, 4000, Germany
SOURCE: Makromolekulare Chemie (1991), 192(8), 1859-72
CODEN: MACEAK; ISSN: 0025-116X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 15 Nov 1991
AB A synthetic route to combined main-chain/side-group chiral liquid-crystalline (lc) polyether-polyesters via precursor polymers containing phenolic side groups is presented. A polymer-analogous reaction with chiral acids (phenol

esterification conversions 90-100%) gives 33 new chiral lc polymers, which exhibit chiral smectic C*, smectic A, and cholesteric phases.

IT 136883-06-2P 136883-07-3P 136883-15-3P
136883-21-1P 136883-25-5P 136883-33-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(liquid-crystalline, preparation and characterization of)

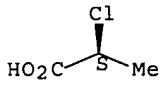
RN 136883-06-2 CAPLUS

CN Propanedioic acid, [6-[(4'-hydroxy[1,1'-biphenyl]-4-yl)oxy]hexyl]-, diethyl ester, polymer with (E)-6,6'-[azobis(4,1-phenyleneoxy)]bis[1-hexanol], (S)-2-chloropropanoate (9CI) (CA INDEX NAME)

CM 1

CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).

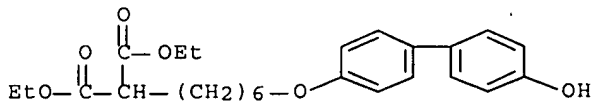


CM 2

CRN 136691-95-7
CMF (C25 H32 O6 . C24 H34 N2 O4)x
CCI PMS

CM 3

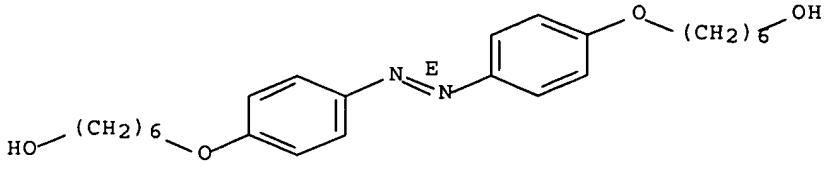
CRN 117823-20-8
CMF C25 H32 O6



CM 4

CRN 109359-32-2
CMF C24 H34 N2 O4

Double bond geometry as shown.

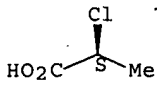


RN 136883-07-3 CAPLUS
CN Propanedioic acid, [6-[(4'-hydroxy[1,1'-biphenyl]-4-yl)oxy]hexyl]-, diethyl ester, polymer with (Z)-6,6'-[azoxybis(4,1-phenyleneoxy)]bis[1-hexanol], (S)-2-chloropropanoate (9CI) (CA INDEX NAME)

CM 1

CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).

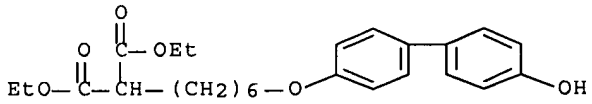


CM 2

CRN 136691-91-3
CMF (C25 H32 O6 . C24 H34 N2 O5)x
CCI PMS

CM 3

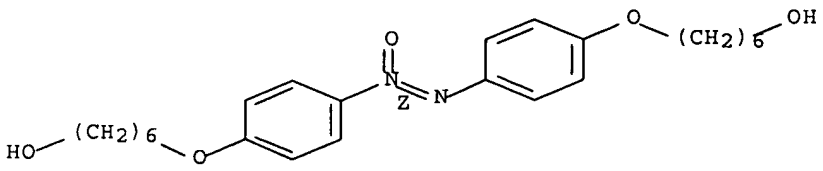
CRN 117823-20-8
CMF C25 H32 O6



CM 4

CRN 114464-39-0
CMF C24 H34 N2 O5

Double bond geometry as shown.



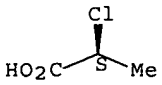
RN 136883-15-3 CAPLUS
CN Propanedioic acid, [6-[(4'-hydroxy[1,1'-biphenyl]-4-yl)oxy]hexyl]-,

diethyl ester, polymer with 6,6'-[[1,1'-biphenyl]-4,4'-diylbis(oxy)]bis[1-hexanol], (S)-2-chloropropanoate (9CI) (CA INDEX NAME)

CM 1

CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).

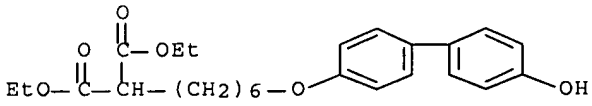


CM 2

CRN 136691-90-2
CMF (C25 H32 O6 . C24 H34 O4)x
CCI PMS

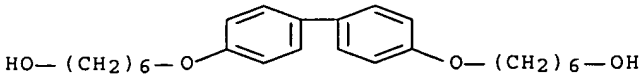
CM 3

CRN 117823-20-8
CMF C25 H32 O6



CM 4

CRN 97087-90-6
CMF C24 H34 O4

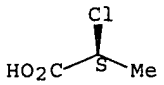


RN 136883-21-1 CAPLUS
CN Propanedioic acid, [6-[(4'-hydroxy[1,1'-biphenyl]-4-yl)oxy]hexyl]-, diethyl ester, polymer with 6,6'-[(3-bromo[1,1'-biphenyl]-4,4'-diyl)bis(oxy)]bis[1-hexanol], (S)-2-chloropropanoate (9CI) (CA INDEX NAME)

CM 1

CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).

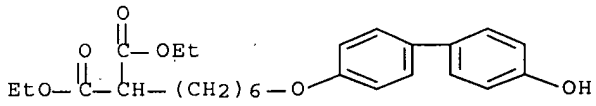


CM 2

CRN 136691-94-6
CMF (C25 H32 O6 . C24 H33 Br O4)x
CCI PMS

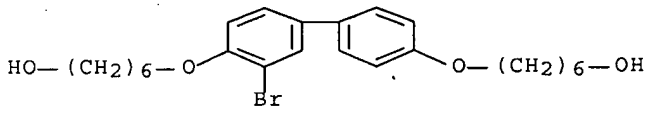
CM 3

CRN 117823-20-8
CMF C25 H32 O6



CM 4

CRN 114464-37-8
CMF C24 H33 Br O4

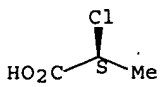


RN 136883-25-5 CAPLUS
CN Propanedioic acid, [6-[4-[(4-hydroxyphenyl)azoxy]phenoxy]hexyl]-, diethyl ester, (Z)-, polymer with (E)-6,6'-[azobis(4,1-phenyleneoxy)]bis[1-hexanol], (S)-2-chloropropanoate (9CI) (CA INDEX NAME)

CM 1

CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 198495-64-6
CMF (C25 H32 N2 O7 . C24 H34 N2 O4)x
CCI PMS

CM 3

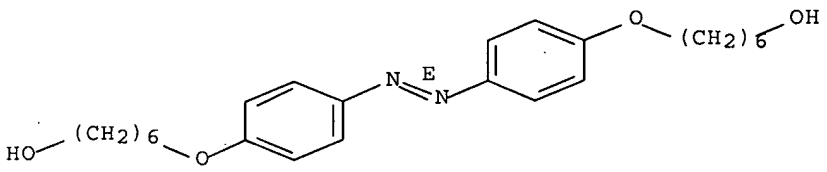
CRN 198495-62-4
CMF C25 H32 N2 O7
CCI IDS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 4

CRN 109359-32-2
CMF C24 H34 N2 O4

Double bond geometry as shown.

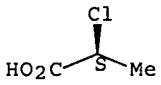


RN 136883-33-5 CAPLUS
CN Propanedioic acid, [6-[4-[(4-hydroxyphenyl)azoxy]phenoxy]hexyl]-, diethyl ester, (Z)-, polymer with 6,6'-[[1,1'-biphenyl]-4,4'-diylbis(oxy)]bis[1-hexanol], (S)-2-chloropropanoate (9CI) (CA INDEX NAME)

CM 1

CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).



CM 2

CRN 198495-65-7
CMF (C25 H32 N2 O7 . C24 H34 O4)x
CCI PMS

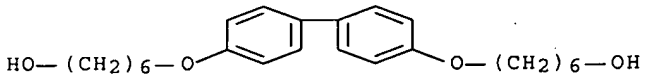
CM 3

CRN 198495-62-4
CMF C25 H32 N2 O7
CCI IDS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

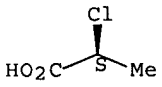
CM 4

CRN 97087-90-6
CMF C24 H34 O4



IT **29617-66-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sp. rotation and esterification of, with polymers containing
phenolic side groups)
RN 29617-66-1 CAPLUS
CN Propanoic acid, 2-chloro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L45 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:206794 CAPLUS Full-text
DOCUMENT NUMBER: 114:206794
TITLE: Preparation of (d)-2-(4-hydroxyphenoxy)propionic acid esters
INVENTOR(S): Nishihira, Keigo; Fujikawa, Shuzo; Hirakawa, Takafumi
PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan; Nissan Chemical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02311444	A	19901227	JP 1989-132894	19890529
JP 2549173	B2	19961030		

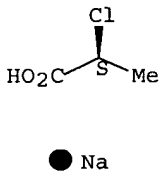
PRIORITY APPLN. INFO.: JP 1989-132894 19890529
ED Entered STN: 31 May 1991
AB (l)-2-Halopropionic acids are treated with hydroquinone or its alkali metal salts in the presence of alkali metal hydroxides in H2O to give an aqueous

solution of (d)-2-(4-hydroxyphenoxy)propionic acid (I) alkali metal salts, which is acidified with acids and extracted with organic solvents to remove the H2O layer, the organic layer is neutralized with aqueous solution of alkali metal hydroxides, separated, and the H2O layer is acidified, concentrated, and cooled, followed by esterification of the preferentially crystallized I in the presence of catalysts to give the title esters useful as intermediates for herbicidal (d)-2-phenoxypropionic acids. An aqueous NaOH solution was added dropwise to (l)-MeCHClCO2Me (95% e.e.) to give an aqueous slurry of (l)-MeCHClCO2Na, which was mixed with an aqueous slurry of p-C6H4(ONa)2 at 30-40 ° for 15 h and kept for 2 h, the reaction mixture was adjusted to pH 1.5 with an aqueous H2SO4 solution and extracted with MIBK twice. The MIBK extract containing I and p-C6H4(CHMeCO2H)2 (II) at the weight ratio 12.6 was diluted with H2O and adjusted to pH 7.5 with an aqueous NaOH solution, then separated, the H2O layer was vacuum-evaporated at 40°, diluted with H2O, and then cooled to 20° to give a wet crystal with I/II weight ratio 89. I thus obtained was esterified with EtOH in toluene containing H2SO4 to give I Et ester with 96.5% chemical purity and 98.5% e.e., vs. 90.6% and 93.2% e.e., resp., for a control obtained by esterification of MIBK extract

IT 74533-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of, with hydroquinone disodium, monoether from)

RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

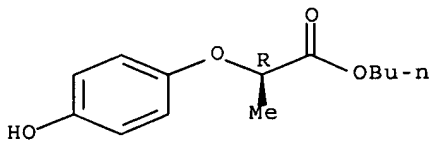
Absolute stereochemistry. Rotation (-).



IT 87129-32-6P 94050-90-5DP, esters 96562-58-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for herbicides)

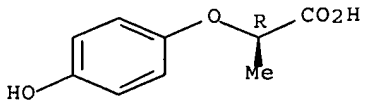
RN 87129-32-6 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, butyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



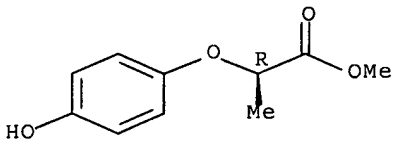
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



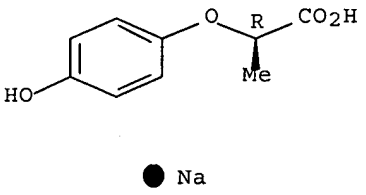
RN 96562-58-2 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



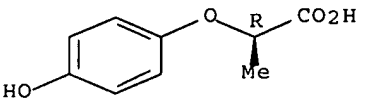
IT 133647-88-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, acidification, and extraction of, free acid from)
RN 133647-88-8 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 94050-90-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, salt formation, and acidification of, and preferential crystallization)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



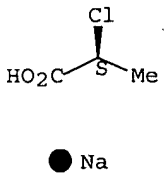
L45 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:440164 CAPLUS Full-text
DOCUMENT NUMBER: 113:40164

TITLE: Preparation of high-purity optically active 2-(4-hydroxyphenoxy)propionic acid
INVENTOR(S): Nishiwaki, Minoru; Hirota, Hideji
PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02032039	A	19900201	JP 1988-181285	19880720
JP 2514072	B2	19960710		

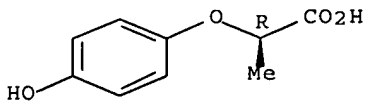
PRIORITY APPLN. INFO.: JP 1988-181285 19880720
ED Entered STN: 03 Aug 1990
AB The title compound (I), useful as an intermediate for herbicides, is prepared in high purity from hydroquinone (II) by successive crystallization of II and I from a crude reaction mixture containing II alkali metal salts and I alkali metal salts. (S)-MeCHClCO2Me was treated with an aqueous NaOH solution and the resulting aqueous solution of (S)-MeCHClCO2Na was added dropwise to a solution of II in an aqueous NaOH solution at 80°, subsequently the reaction mixture was cooled at 5° and adjusted to pH 7 to recover 72.3% II, while the filtrate was adjusted to pH 1 to give 84.7% (R)-I of 98.4% e.e. Further recrystn. in H2O gave (R)-I of 100% e.e.
IT **74533-11-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with hydroquinone sodium, (hydroxyphenoxy)propionic acid from)
RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **94050-90-5P**, (R)-2-(4-Hydroxyphenoxy)propionic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for herbicides)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

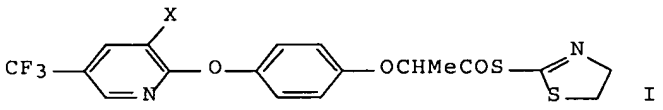
Absolute stereochemistry. Rotation (+).



L45 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:548900 CAPLUS Full-text
DOCUMENT NUMBER: 111:148900
TITLE: Optically-active propionic acid thiazolinyl thioester derivatives as selective herbicides
INVENTOR(S): Ito, Mikio; Watanabe, Hiroyuki; Tsuzuki, Kenji; Someya, Shinzo; Kora, Seigo
PATENT ASSIGNEE(S): Agro-Kanesho Co., Ltd., Japan; Tosoh Corp.
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01050882	A	19890227	JP 1987-207173	19870820

PRIORITY APPLN. INFO.: JP 1987-207173 19870820
OTHER SOURCE(S): MARPAT 111:148900
ED Entered STN: 28 Oct 1989
GI

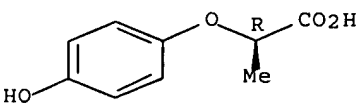


I

AB The title derivs. (R)-I (X = H, Cl) are prepared A solution of 0.84 g 2-mercaptothiazoline in CH2Cl2 was treated with 2.97 g (R)-(+)-2-[4-(3-chloro-5-trifluoromethyl-2-pyridyloxy)phenoxy]propionyl chloride (preparation given) at room temperature to give 1.9 g (R)-I (X = Cl) (II). An emulsion was formulated from II 20, xylene 60, and Sorpol 2806B 20 parts. II, at 0.2 g/are, showed complete control of barnyard grass, Digitaria adscendens, and Avena sativa, without any damage to crops in pot expts., vs., poor control using racemic II.

IT 94050-90-5P, (R)-(+)-2-(4-Hydroxyphenoxy)propionic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with chlorotrifluoromethylpyridine derivs.)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

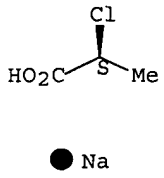
Absolute stereochemistry. Rotation (+).



IT 74533-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with hydroquinone)
RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

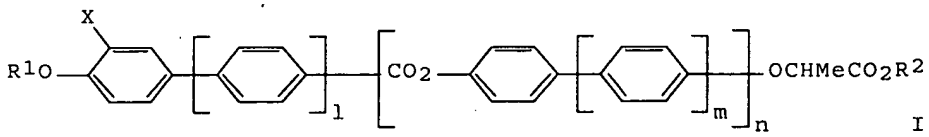
Absolute stereochemistry. Rotation (-).



L45 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:523975 CAPLUS Full-text
DOCUMENT NUMBER: 111:123975
TITLE: Phenoxypropionate ester derivatives for ferroelectric liquid-crystal display devices
INVENTOR(S): Shoji, Tadao; Takehara, Sadao; Fujisawa, Noburu; Ogawa, Hiroshi; Osawa, Masashi
PATENT ASSIGNEE(S): Dainippon Ink and Chemicals, Inc., Japan; Kawamura Physical and Chemical Research Institute
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01042455	A	19890214	JP 1987-198152	19870810
PRIORITY APPLN. INFO.:			JP 1987-198152	19870810

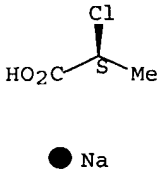
OTHER SOURCE(S): MARPAT 111:123975
ED Entered STN: 01 Oct 1989
GI



AB The title derivs. I (R1 = C≤20 n-alkyl; R2 = C≤20 n-alkyl, optically-active alkyl; X = H, halo; l, m, n = 0, 1; n = 1 when l = 0; n = 0 when l = 1) are claimed. I or liquid-crystal compns. containing I show a chiral smectic C phase at a wide range of temperature and are useful for display devices with a quick response. Successive treatment of (R)-ClCHMeCO2Na with 4,4'-biphenol and (S)-(-)-EtCHMeCH2OH gave (S,S)-4- HOC6H4C6H4OCHMeCO2CH2CHMeEt-4, which was treated with 4-Me(CH2)7OC6H4COCl to give (S,S)-I (R1 = octyl; R2 = CH2CHMeEt; l = 0; m = n = 1) (II). A mixture of II and 4-Me(CH2)9OC6H4CO2C6H4O(CH2)7Me-4 having no chiral smectic phase showed a chiral smectic C phase.

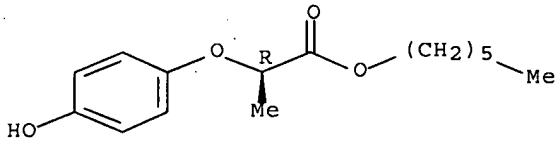
IT 74533-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with hydroquinone or biphenols, in preparation
of liquid crystals)
RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



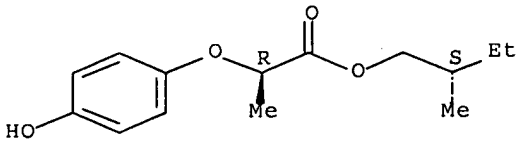
IT 113918-70-0P 122330-44-3P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, with benzoyl chloride in preparation of liquid
crystal)
RN 113918-70-0 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, hexyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



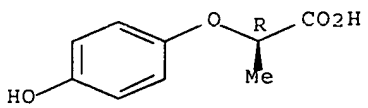
RN 122330-44-3 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, 2-methylbutyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 94050-90-5P, (R)-2-(4-Hydroxyphenoxy)propionic acid
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, with methylbutanol or hexanol, in preparation
of liquid crystals)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

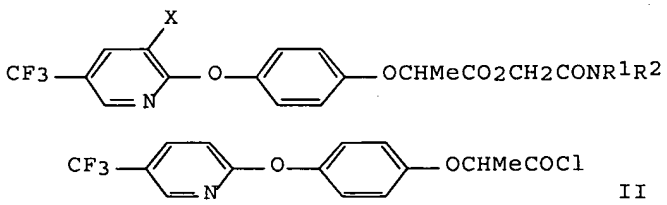
Absolute stereochemistry. Rotation (+).



L45 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:553635 CAPLUS Full-text
DOCUMENT NUMBER: 111:153635
TITLE: Preparation of optically active α-[2-[4-(trifluoromethyl-2-pyridyloxy)phenoxy]propionyloxy]acetamide derivatives as herbicides
INVENTOR(S): Someya, Shinzo; Kora, Seigo; Ito, Mikio; Watanabe, Hiroyuki; Tsuzuki, Kenji
PATENT ASSIGNEE(S): Agro-Kanesho Co., Ltd., Japan; Tosoh Corp.
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01009975	A	19890113	JP 1987-165972	19870702
PRIORITY APPLN. INFO.:			JP 1987-165972	19870702

OTHER SOURCE(S): MARPAT 111:153635
ED Entered STN: 28 Oct 1989
GI

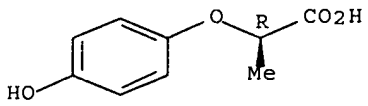


I

II

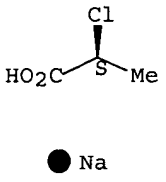
AB The title compds. [(R)-I; R1, R2 = Me, MeO, methoxyethyl; X = H, halo], useful as selective herbicides, are prepared Optically active propionyl chloride (R)-II (preparation given) was reacted with HOCH2CONMeOMe in CH2Cl2 containing Et3N to give (R)-I (X = H, R1 = Me, R2 = MeO) [(R)-II]. At 0.4 g/a (R)-II was more effective than (±)-II in controlling barnyard grass.
IT **94050-90-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of herbicides)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



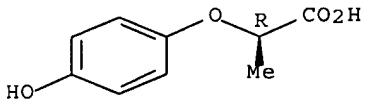
IT 74533-11-2 94050-90-5, (R)-2-(4-Hydroxyphenoxy)propionic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of herbicides)
RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L45 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:446353 CAPLUS Full-text
DOCUMENT NUMBER: 109:46353
TITLE: Ferroelectric liquid-crystal compounds for display devices
INVENTOR(S): Jackson, David Anthony; Gemmell, Peter Alan
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 259995	A1	19880316	EP 1987-307355	19870820
EP 259995	B1	19901017		

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

AT 57524	T	19901115	AT 1987-307355		19870820
US 4906402	A	19900306	US 1987-91895		19870901
JP 63077840	A	19880408	JP 1987-223221		19870908
PRIORITY APPLN. INFO.:			GB 1986-21689	A	19860909
			EP 1987-307355	A	19870820

ED Entered STN: 05 Aug 1988

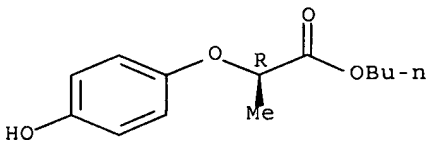
AB The compds. are preferably CpH2p+1OA1A2TA3Z1CH(Me)CO2CqH2q+1, where p = 6-12; q = 2-12; Z1 = O or S; T = COO or COS; and A1, A2, A3 = 1,4-phenylene, 1,4-cyclohexylene (optionally with 1 or 2 C atoms replaced by O or S), 1,4-bicyclo-[2.2.2]octane, 1,6-naphthylene, or 1,4-naphthylene, unsubstituted or F-substituted. (R)-2-(4- Hydroxyphenoxy)propionic acid was esterified with 1-pentanol, and 4-(4-octyloxyphenyl)benzoic acid was converted into its acid chloride. The ester and the acid chloride were reacted to form pentyl (R)-2-(4-[4-(4-octyloxyphenyl)benzoyloxy]phenoxy)propanoate, m. 55° and having sp. optical rotation +16° at 589 nm and 20-25° in CHCl3.

IT **87129-32-6P 94050-90-5P 96562-58-2P**
113918-70-0P 114755-07-6P 114755-10-1P
114755-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in formation of ferroelec. liquid crystals for
display devices)

RN 87129-32-6 CAPLUS

CN Propanoic acid, 2-(4-hydroxyphenoxy)-, butyl ester, (2R)- (9CI) (CA INDEX NAME)

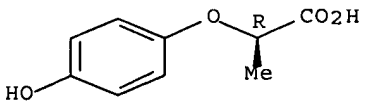
Absolute stereochemistry. Rotation (+).



RN 94050-90-5 CAPLUS

CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

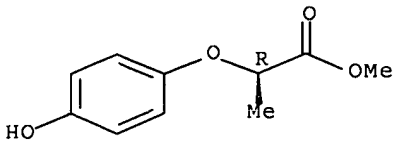
Absolute stereochemistry. Rotation (+).



RN 96562-58-2 CAPLUS

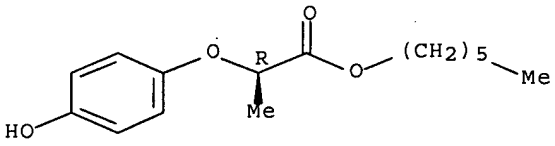
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



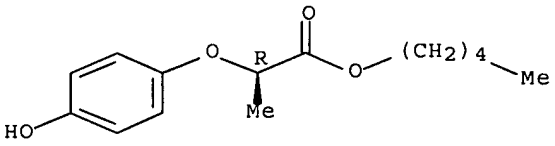
RN 113918-70-0 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, hexyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



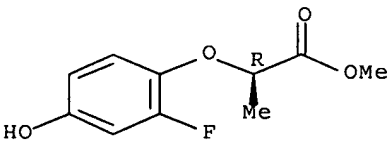
RN 114755-07-6 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, pentyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



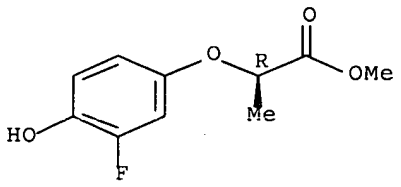
RN 114755-10-1 CAPLUS
CN Propanoic acid, 2-(2-fluoro-4-hydroxyphenoxy)-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



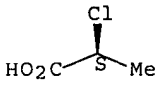
RN 114755-11-2 CAPLUS
CN Propanoic acid, 2-(3-fluoro-4-hydroxyphenoxy)-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



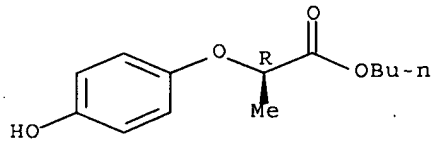
IT 29617-66-1 87129-32-6 94050-90-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in formation of ferroelec. liquid crystals for display devices)
RN 29617-66-1 CAPLUS
CN Propanoic acid, 2-chloro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



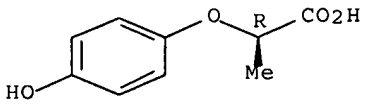
RN 87129-32-6 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, butyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



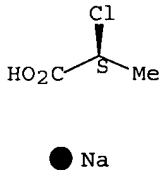
L45 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:439415 CAPLUS Full-text
DOCUMENT NUMBER: 107:39415
TITLE: Optically active 2-(4-hydroxyphenoxy)propionic acid as herbicide intermediate
INVENTOR(S): Suzuki, Kenji; Hashiba, Isao; Tsuchiya, Shuji; Takakuwa, Yasuo
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62016446	A	19870124	JP 1984-225327	19841026
JP 06010153	B	19940209		

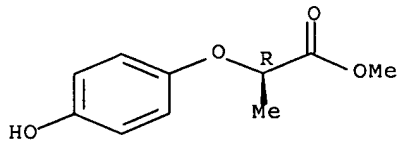
PRIORITY APPLN. INFO.: JP 1984-225327 19841026
ED Entered STN: 08 Aug 1987
AB The title acid (I), useful as an intermediate for herbicides, is prepared An EtOH solution of 1-MeCHClCO2Na, obtained from 85.8 g 1-MeCHClCO2Me and NaOH, was heated with 110 g p-HOC6H4OH (II) and NaOH at 60°, and refluxed in C6H6 to give 130 g d-I Et ester having 93% enantiomeric excess.
IT 74533-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with hydroquinone)
RN 74533-11-2 CAPLUS
CN Propanoic acid, 2-chloro-, sodium salt, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 96562-58-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as herbicide intermediate)
RN 96562-58-2 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L45 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:66753 CAPLUS Full-text
DOCUMENT NUMBER: 106:66753
TITLE: Optical resolution of (±)-2-chloropropionic acid
INVENTOR(S): Nohira, Hiroyuki; Endo, Koji; Nishiyama, Takahito
PATENT ASSIGNEE(S): Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

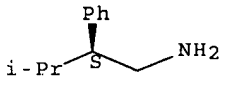
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61172846	A	19860804	JP 1985-15203	19850129

PRIORITY APPLN. INFO.: JP 1985-15203 19850129
ED Entered STN: 07 Mar 1987
AB (+)- Or (-)-2-chloropropionic acid [(+)- or (-)-I], useful as intermediate for optically active alanine and lactic acid, were prepared by optical resolution of (±)-I by treating with optically active p- RC6H4CH(CHMe2)CH2NH2 (II; R = H, Me). Thus, (±)-I and (+)-II (R = H) (III) were heated, then (-)-I, (+)-III salt was added and left at room temperature for 5 h to give 31.5% (-)-I, (+)-II salt, which was treated with aqueous NaOH to give 24.2% (-)-I in 83.2% optical purity.
IT **106498-33-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of)
RN 106498-33-3 CAPLUS
CN Propanoic acid, 2-chloro-, (S)-, compd. with (S)-β-(1-methylethyl)benzeneethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 106498-32-2
CMF C11 H17 N

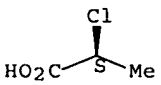
Absolute stereochemistry. Rotation (+).



CM 2

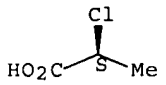
CRN 29617-66-1
CMF C3 H5 Cl O2

Absolute stereochemistry. Rotation (-).



IT **29617-66-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for optically active alanine and lactic acid)
RN 29617-66-1 CAPLUS
CN Propanoic acid, 2-chloro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CLAIM 7

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FILE 'CAPLUS' ENTERED AT 10:48:37 ON 18 DEC 2006
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FILE COVERS 1907 - 18 Dec 2006  VOL 145 ISS 26
FILE LAST UPDATED: 17 Dec 2006  (20061217/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE


L3              1 SEA FILE=REGISTRY ABB=ON  72619-32-0
L4              1 SEA FILE=REGISTRY ABB=ON  114420-56-3
L6              1 SEA FILE=REGISTRY ABB=ON  FLUAZIFOP-P-BUTYL/CN
L10             1 SEA FILE=REGISTRY ABB=ON  CYHALOFOP-BUTYL/CN
L11             1 SEA FILE=REGISTRY ABB=ON  QUIZALOFOP-P-ETHYL/CN
L12             1 SEA FILE=REGISTRY ABB=ON  71283-80-2
L13             6 SEA FILE=REGISTRY ABB=ON  (L11 OR L3 OR L6 OR L4 OR L10 OR
                  L12)
L14            28 SEA FILE=CAPLUS ABB=ON  L13/P
L17               STR
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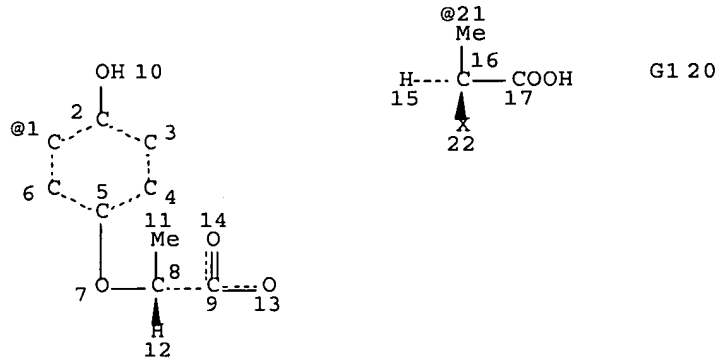


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  20

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 2
L19           72 SEA FILE=REGISTRY SSS FUL L17
L20           49 SEA FILE=REGISTRY ABB=ON  46.150.18/RID AND L19
L23          115 SEA FILE=CAPLUS ABB=ON  L20
L25           11 SEA FILE=CAPLUS ABB=ON  L23 AND L14


=> s l25 not l43,l40
L46          10 L25 NOT (L43 OR L40)

=> fil casreact; d stat que l36
FILE 'CASREACT' ENTERED AT 10:48:57 ON 18 DEC 2006
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FILE CONTENT:1840 - 17 Dec 2006 VOL 145 ISS 25

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*****************************************************************
*                                                               *
*     CASREACT now has more than 10 million reactions           *
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*****************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.


L34             STR
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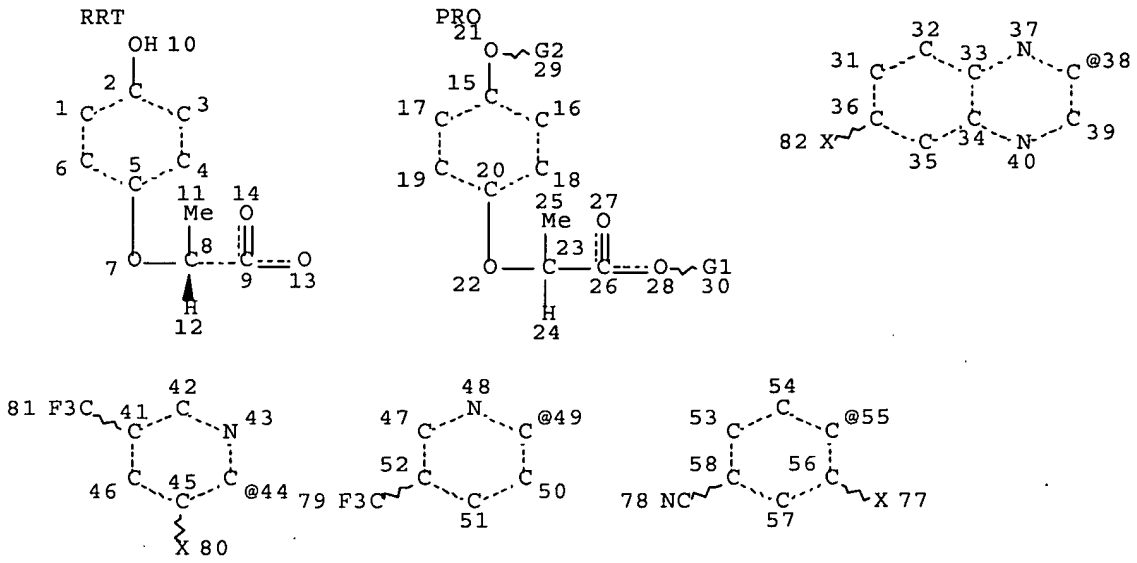
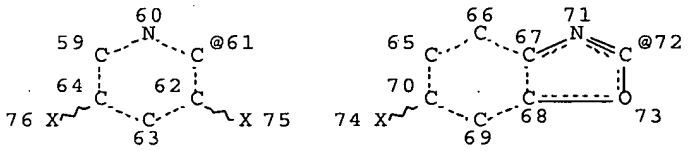


Page 1-A



Page 2-A
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 82

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1
L36 19 SEA FILE=CASREACT SSS FUL L34 (70 REACTIONS)

100.0% DONE 424 VERIFIED 70 HIT RXNS 19 DOCS
SEARCH TIME: 00.00.01

=> s l36 not l44,l41
L47 19 L36 NOT (L44 OR L41)

=> dup rem l47,l46
FILE 'CASREACT' ENTERED AT 10:49:28 ON 18 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE 'CAPLUS' ENTERED AT 10:49:28 ON 18 DEC 2006
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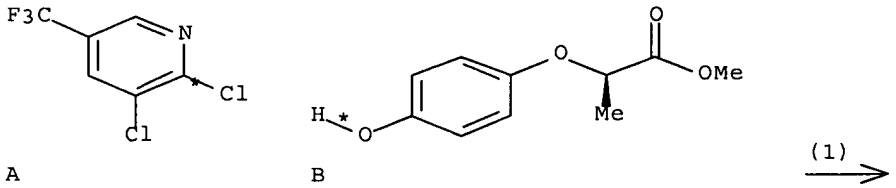
PROCESSING COMPLETED FOR L47
PROCESSING COMPLETED FOR L46
L48 27 DUP REM L47 L46 (2 DUPLICATES REMOVED)
ANSWERS '1-19' FROM FILE CASREACT
ANSWERS '20-27' FROM FILE CAPLUS

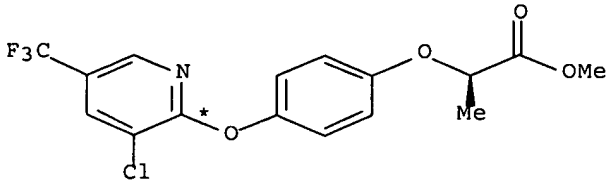
=> d ibib abs hit 1-19; d ibib ed abs hitstr 20-27; fil hom

L48 ANSWER 1 OF 27 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 144:412325 CASREACT Full-text
TITLE: Synthesis of R-(+)-Haloxyfop-methyl
AUTHOR(S): Yan, Xin; Song, Meng; Lin, Zhou; Wang, Zun-yao
CORPORATE SOURCE: Department of Chemical Engineering, Yancheng Institute of Technology, Yancheng, 224003, Peop. Rep. China
SOURCE: Jiangsu Huagong (2004), 32(4), 26-28, 33
CODEN: JHIUAC; ISSN: 1002-1116
PUBLISHER: Jiangsusheng Huagong Xinxi Zhongxin
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Title compound was prepared by the etherification of R-(+)-Me 2-(4-hydroxyphenoxy)propionate and 2,3-dichloro-5-trifluoromethylpyridine with the presence of tetrabutylammonium bromide as phase transfer catalyst and powdered anhydrous potassium carbonate as bounding acid, provided product with yield 88%. The product was characterized by IR, 1H NMR, GC-MS and polarimetry.

RX(1) OF 1 A + B ===> C



A B



C
YIELD 88%

RX(1) RCT A 69045-84-7

STAGE(1)
RGT D 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON 1.5 hours, room temperature

STAGE(2)
RCT B 96562-58-2
CAT 1643-19-2 Bu4N.Br
SOL 67-68-5 DMSO
CON 37 hours, room temperature

PRO C 72619-32-0
NTE regioselective, phase transfer catalyst used, optimization study, yield depends on the kind of solvents, the amount of catalyst, the reaction time

L48 ANSWER 2 OF 27 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 113:77920 CASREACT Full-text
TITLE: An improved process for the minimization of racemization in the preparation of optically active [(aryloxy)phenoxy]propionate herbicides
INVENTOR(S): Kershner, Larry D.; Tai, Jimmy J.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 344746	A2	19891206	EP 1989-109844	19890531
EP 344746	A3	19911127		
EP 344746	B1	19941221		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4897481	A	19900130	US 1988-200400	19880531
CA 1327804	C	19940315	CA 1989-601119	19890530
IL 90460	A	19941128	IL 1989-90460	19890530
AU 8935876	A	19891207	AU 1989-35876	19890531
AU 614620	B2	19910905		
WO 8912043	A1	19891214	WO 1989-US2378	19890531
W: BR, DK, JP, SU				
BR 8906997	A	19901218	BR 1989-6997	19890531
JP 02504639	T	19901227	JP 1989-506598	19890531
JP 2878360	B2	19990405		
DK 9000253	A	19900130	DK 1990-253	19900130
DK 175378	B1	20040920		
SU 1811521	A3	19930423	SU 1990-4743141	19900130
PRIORITY APPLN. INFO.:			US 1988-200400	19880531
			WO 1989-US2378	19890531

OTHER SOURCE(S): MARPAT 113:77920
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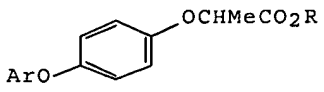
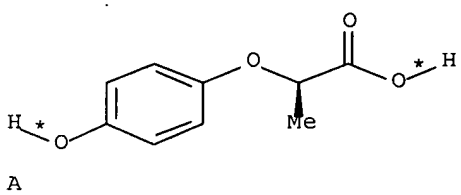


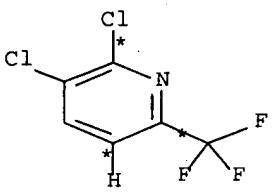
I

AB The process for reducing the amount of racemization in preparation of title compds. I (Ar = aryl activated toward aromatic nucleophilic substitution; R = C1-8 alkyl, C3-8 alkoxyalkyl) is characterized by reacting an alkali metal salt of an appropriate phenoxypropionic acid with ArX (X = halo). (R)-4-HOC6H4OCHMeCO2H (9.2 g; R/S = 97/3) and 3,4-F2C6H3CN in DMSO were reacted with K2CO3 at 85° and kept for 2 h to give (R)-I [Ar = 4,2-(NC)FC6H3; R = H] which was converted to (R)-I [Ar = 4,2-(NC)FC6H3; R = Me] (R/S ratio 97/3).

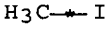
RX(1) OF 2 **A** + **B** + **C** ===> **D**



A



B



C

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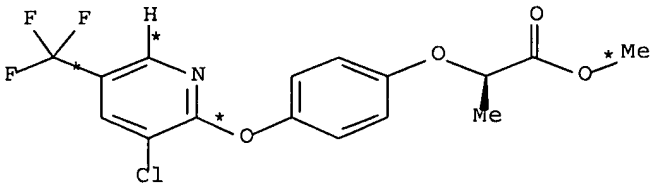
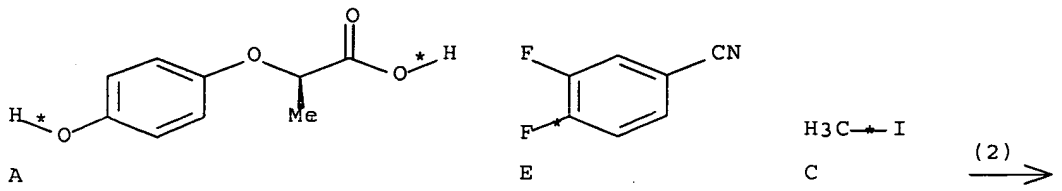


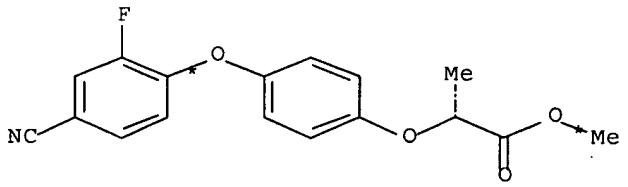
D

RX(1) RCT A 94050-90-5, B 89719-90-4, C 74-88-4
PRO D 72619-32-0

RX(2) OF 2 **A** + **E** + **C** ===> **F**



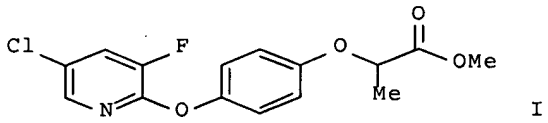
A E C



F

RX(2) RCT A 94050-90-5, E 64248-62-0, C 74-88-4
PRO F 122088-57-7

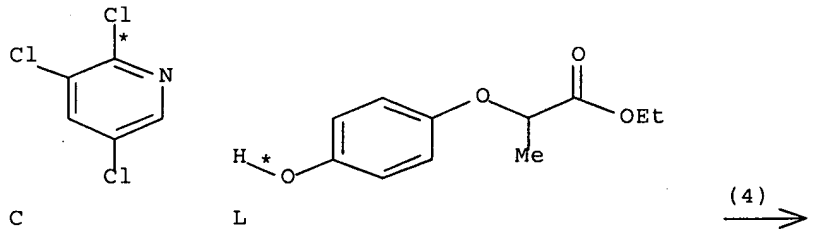
L48 ANSWER 3 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:134429 CASREACT Full-text
TITLE: Direct Formation of 2,3,5-Trichloropyridine and its Nucleophilic Displacement Reactions in Ionic Liquid
AUTHOR(S): Zhong, Ping; Hu, Huanan; Guo, Shengrong
CORPORATE SOURCE: Department of Chemistry, Wenzhou Normal College, Wenzhou, Peop. Rep. China
SOURCE: Synthetic Communications (2004), 34(23), 4301-4311
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



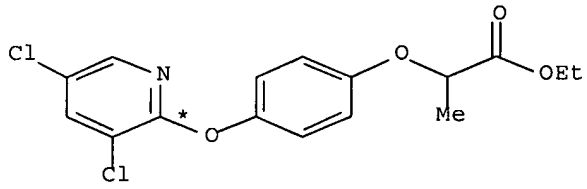
I

AB Reaction of trichloroacetaldehyde and acrylonitrile in the presence of a catalytic amount of copper (I) chloride in ionic liquid afforded 2,3,5-trichloropyridine, fluorination of which with KF and CsF in ionic liquid afforded 3,5-dichloro-2-fluoro- and 5-chloro-2,3-dichloropyridines. Reaction of 2,3,5-trichloro-, 3,5-dichloro-2-fluoro-, or 5-chloro-2,3-dichloropyridine with 2-(4-hydroxyphenoxy)propionates in ionic liquid afforded the corresponding 2-aryloxylpropionates, e.g., I, in good yields.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 44 ...C + L ===> M



C L (4)



M
YIELD 75%

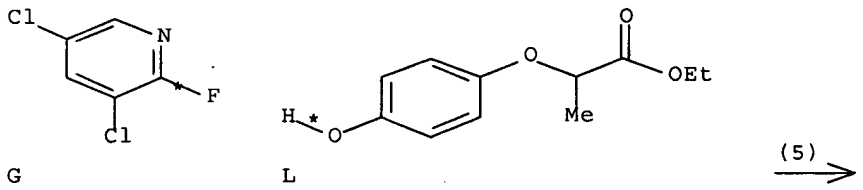
RX(4) RCT C 16063-70-0, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

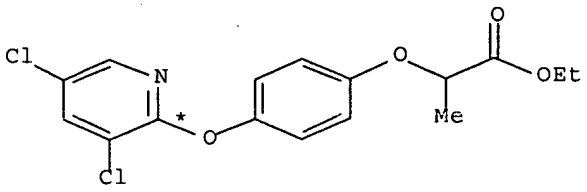
STAGE(2)
SOL 7732-18-5 Water

PRO M 60074-47-7

RX(5) OF 44 ...G + L ===> M



G L (5)



M
YIELD 82%

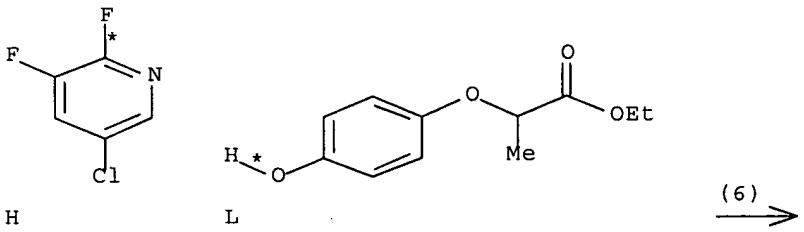
RX(5) RCT G 823-56-3, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

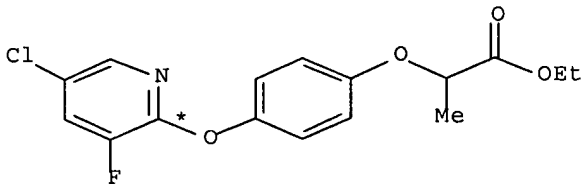
STAGE(2)
SOL 7732-18-5 Water

PRO M 60074-47-7

RX(6) OF 44 ...H + L ===> O



H L (6)



O
YIELD 81%

RX(6) RCT H 89402-43-7, L 65343-67-1

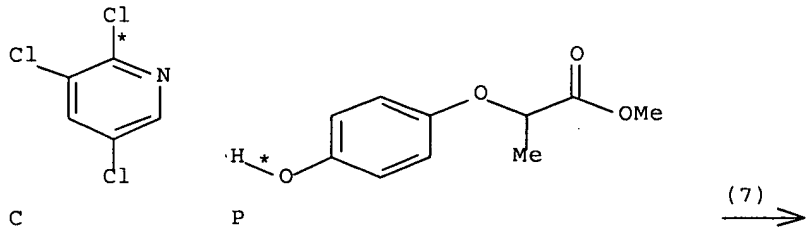
STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3

SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

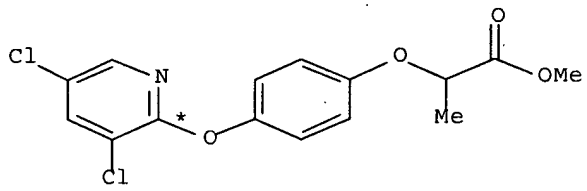
STAGE(2)
SOL 7732-18-5 Water

PRO O 105511-94-2

RX(7) OF 44 ...C + P ===> Q



C P



Q
YIELD 77%

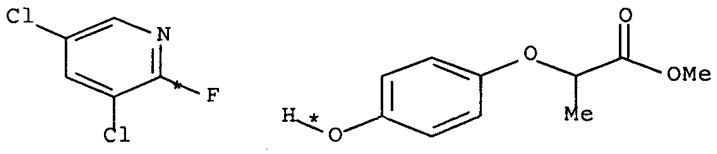
RX(7) RCT C 16063-70-0, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

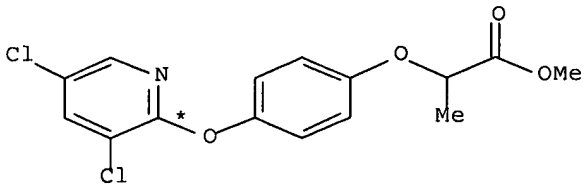
STAGE(2)
SOL 7732-18-5 Water

PRO Q 60074-46-6

RX(8) OF 44 ...G + P ===> Q



G P (8)



Q
YIELD 85%

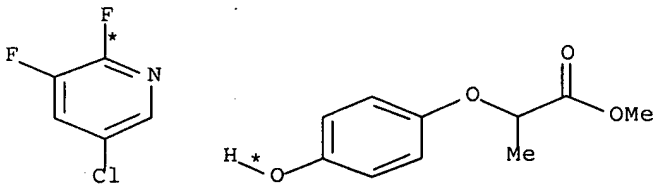
RX(8) RCT G 823-56-3, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

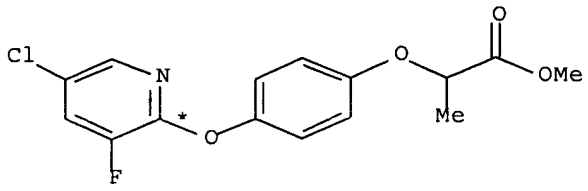
STAGE(2)
SOL 7732-18-5 Water

PRO Q 60074-46-6

RX(9) OF 44 ...H + P ===> R...



H P (9)



R
YIELD 80%

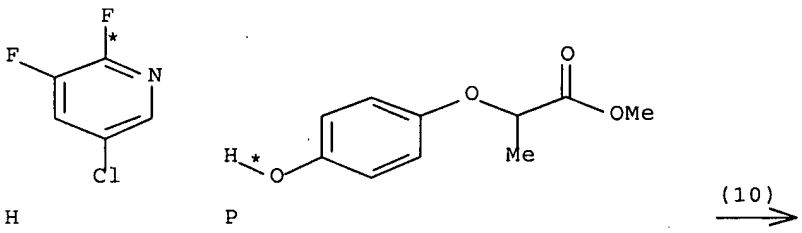
RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

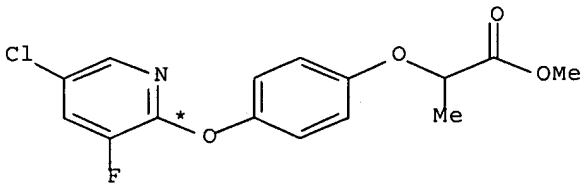
STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

RX(10) OF 44 H + P ===> R



H P (10)



R
YIELD 70%

RX(10) RCT H 89402-43-7, P 60075-04-9

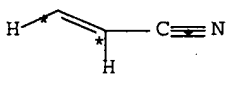
STAGE(1)
RGT I 584-08-7 K2CO3
SOL 75-05-8 MeCN

CON 40 hours, 50 - 60 deg C

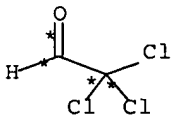
STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

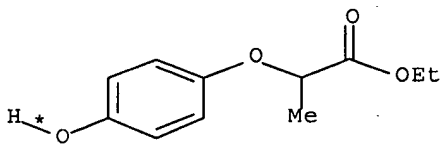
RX(17) OF 44 COMPOSED OF RX(1), RX(4)
RX(17) A + B + L ===> M



A

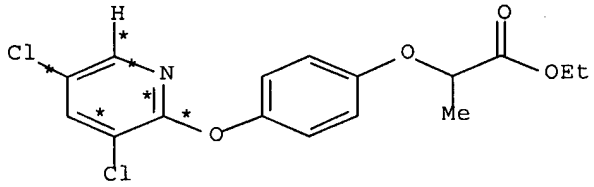


B



L

2 STEPS



M
YIELD 75%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

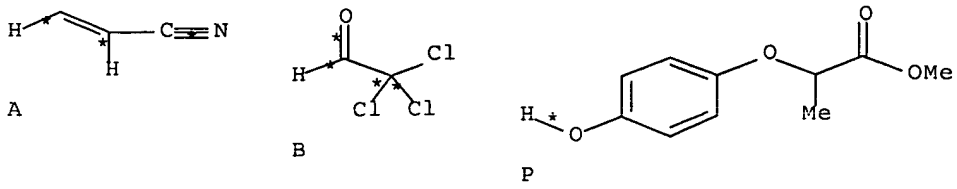
RX(4) RCT C 16063-70-0, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

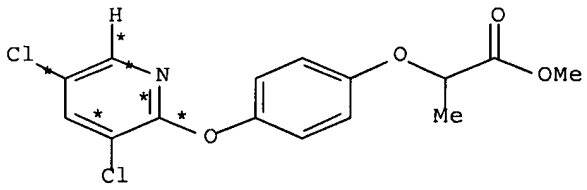
PRO M 60074-47-7

RX(18) OF 44 COMPOSED OF RX(1), RX(7)
RX(18) A + B + P ===> Q



A B P

2 STEPS



Q
YIELD 77%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

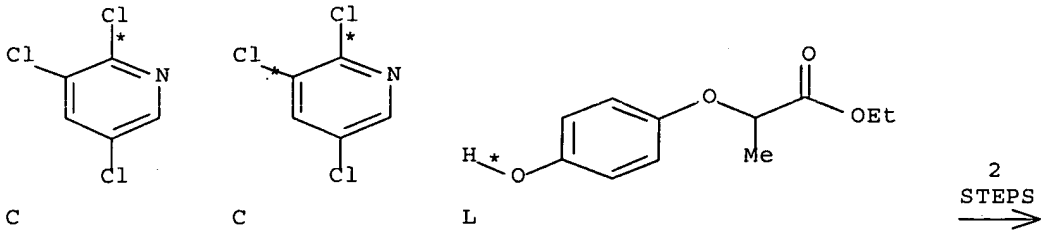
RX(7) RCT C 16063-70-0, P **60075-04-9**

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

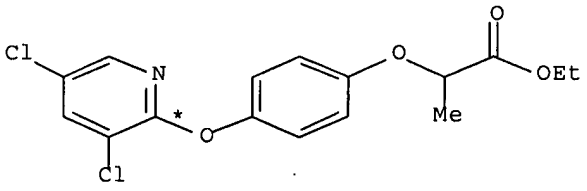
STAGE(2)
SOL 7732-18-5 Water

PRO Q **60074-46-6**

RX(24) OF 44 COMPOSED OF RX(2), RX(5)
RX(24) 2 C + L ===> M



C C L



M
YIELD 82%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

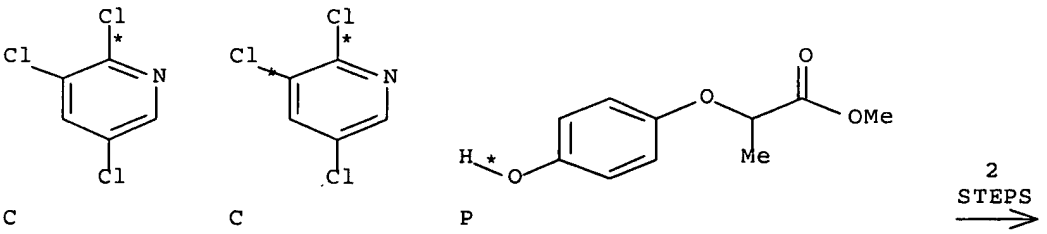
RX(5) RCT G 823-56-3, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

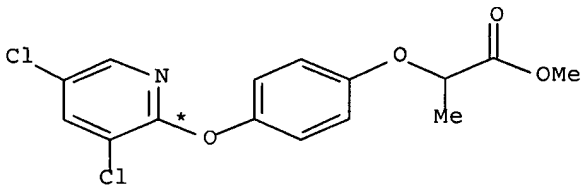
STAGE(2)
SOL 7732-18-5 Water

PRO M 60074-47-7

RX(25) OF 44 COMPOSED OF RX(2), RX(8)
RX(25) 2 C + P ===> Q



C C P



Q
YIELD 85%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

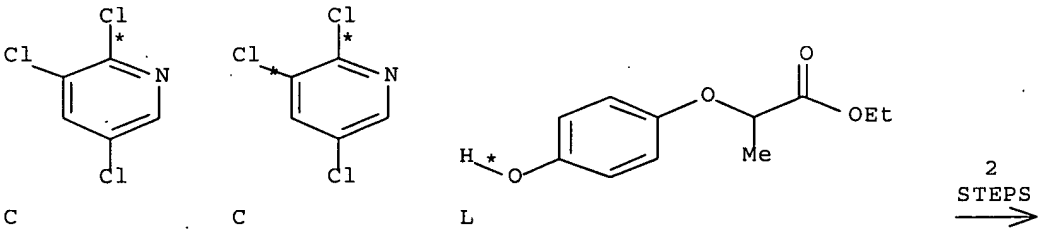
RX(8) RCT G 823-56-3, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

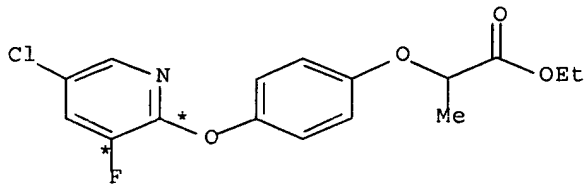
STAGE(2)
SOL 7732-18-5 Water

PRO Q 60074-46-6

RX(26) OF 44 COMPOSED OF RX(2), RX(6)
RX(26) 2 C + L ===> O



C C L 2 STEPS



O
YIELD 81%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

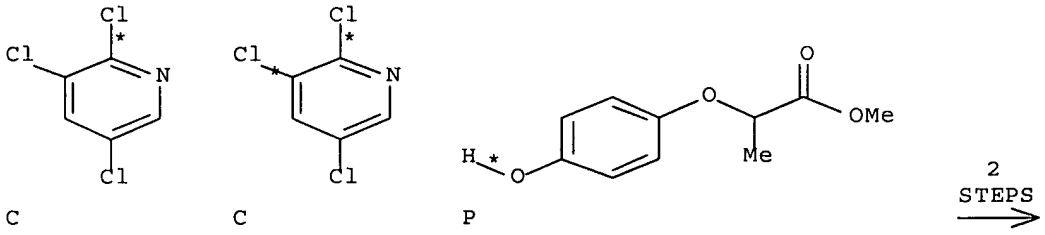
RX(6) RCT H 89402-43-7, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

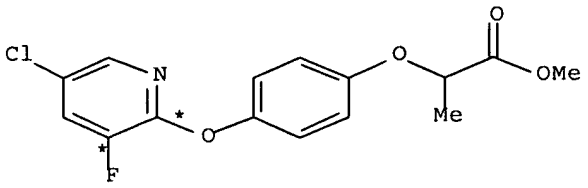
STAGE(2)
SOL 7732-18-5 Water

PRO O 105511-94-2

RX(27) OF 44 COMPOSED OF RX(2), RX(9)
RX(27) 2 C + P ===> R



C C P 2 STEPS



R
YIELD 80%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

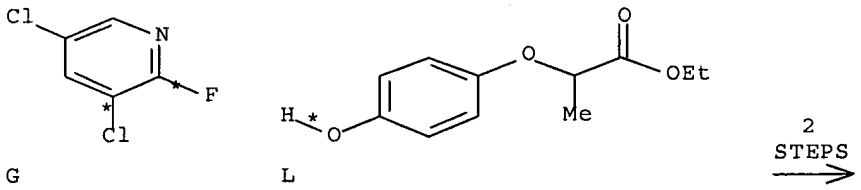
RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

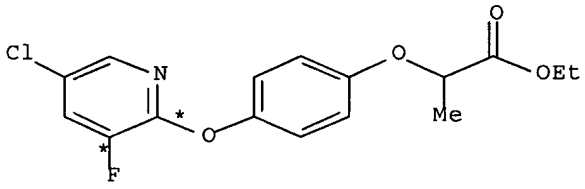
STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

RX(28) OF 44 COMPOSED OF RX(3), RX(6)
RX(28) G + L ===> O



G L



O
YIELD 81%

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

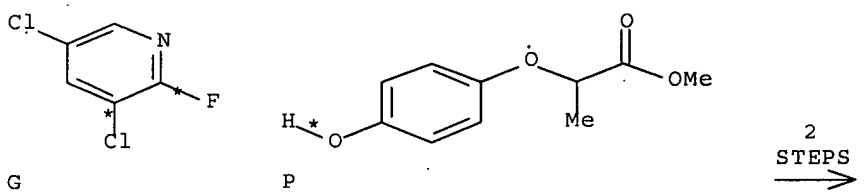
RX(6) RCT H 89402-43-7, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

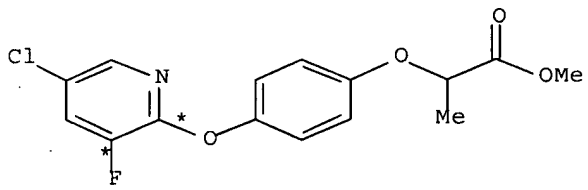
STAGE(2)
SOL 7732-18-5 Water

PRO O **105511-94-2**

RX(29) OF 44 COMPOSED OF RX(3), RX(9)
RX(29) G + P ===> R



G P



R
YIELD 80%

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

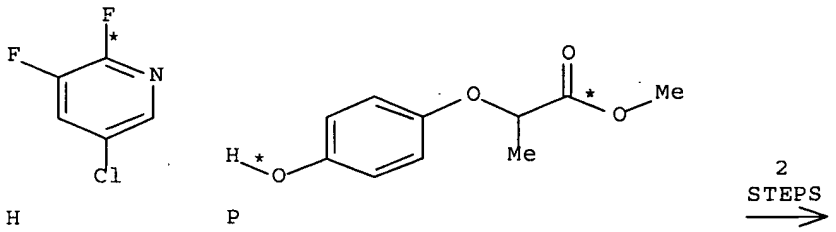
RX(9) RCT H 89402-43-7, P **60075-04-9**

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

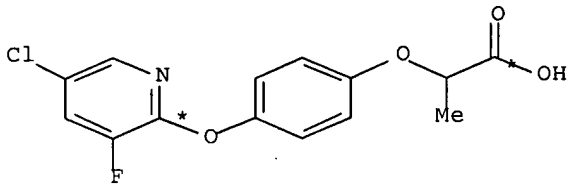
STAGE(2)
SOL 7732-18-5 Water

PRO R **87035-49-2**

RX(30) OF 44 COMPOSED OF RX(9), RX(15)
RX(30) H + P ===> AA



H P



AA
YIELD 82%

RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

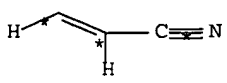
RX(15) RCT R 87035-49-2

STAGE(1)
RGT AB 1310-73-2 NaOH
SOL 123-91-1 Dioxane
CON 3 hours, 35 deg C

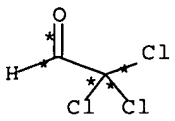
STAGE(2)
RGT AC 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AA 87135-08-8

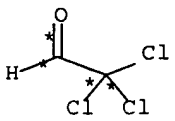
RX(32) OF 44 COMPOSED OF RX(1), RX(2), RX(5)
RX(32) 2 A + 2 B + L ===> M



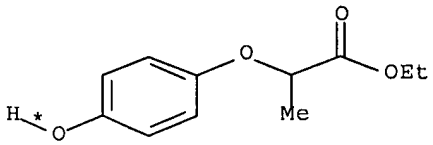
2 A



B

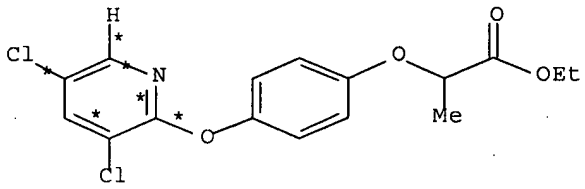


B



L

3
STEPS



M
YIELD 82%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

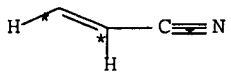
RX(5) RCT G 823-56-3, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

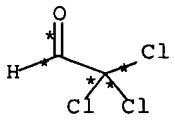
STAGE(2)
SOL 7732-18-5 Water

PRO M 60074-47-7

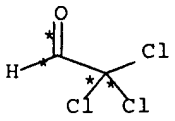
RX(33) OF 44 COMPOSED OF RX(1), RX(2), RX(8)
RX(33) 2 A + 2 B + P ===> Q



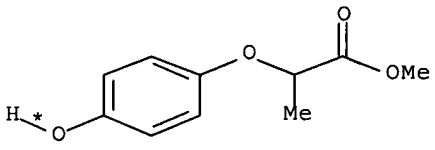
2 A



B

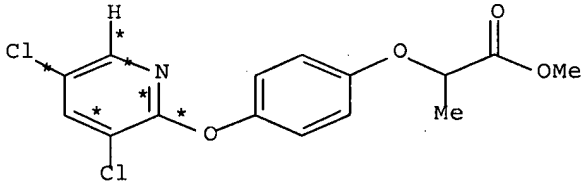


B



P

3
STEPS



Q
YIELD 85%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(8) RCT G 823-56-3, P 60075-04-9

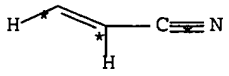
STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3

SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

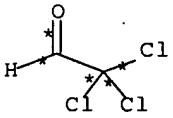
STAGE(2)
SOL 7732-18-5 Water

PRO Q 60074-46-6

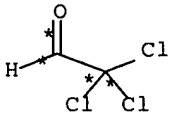
RX(34) OF 44 COMPOSED OF RX(1), RX(2), RX(6)
RX(34) 2 A + 2 B + L ===> O



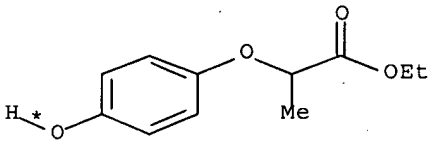
2 A



B

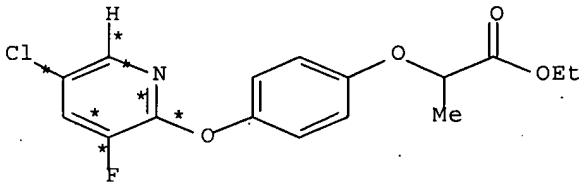


B



L

3
STEPS



O
YIELD 81%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

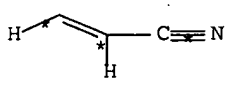
RX(6) RCT H 89402-43-7, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

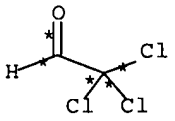
STAGE(2)
SOL 7732-18-5 Water

PRO O 105511-94-2

RX(35) OF 44 COMPOSED OF RX(1), RX(2), RX(9)
RX(35) 2 A + 2 B + P ===> R



2 A



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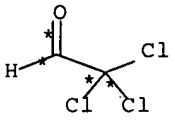
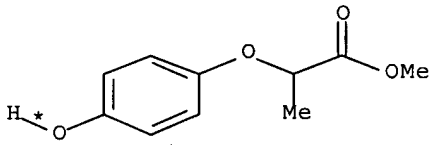
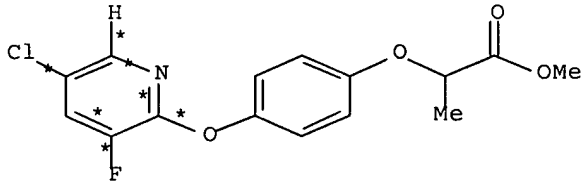


B



P

3 STEPS



R
YIELD 80%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

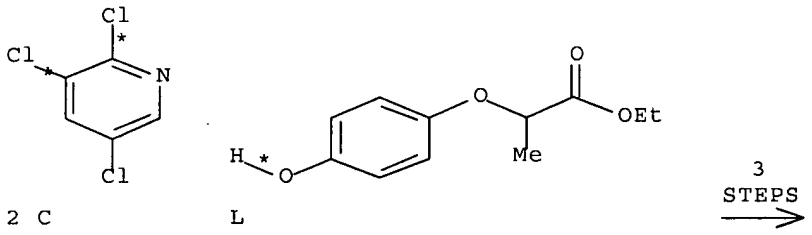
RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

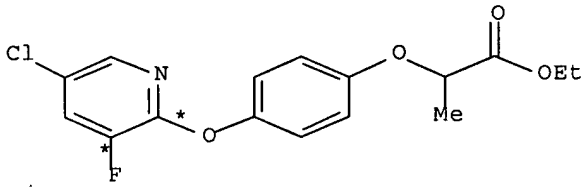
STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

RX(36) OF 44 COMPOSED OF RX(2), RX(3), RX(6)
RX(36) 2 C + L ===> O



2 C L



O
YIELD 81%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7

SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

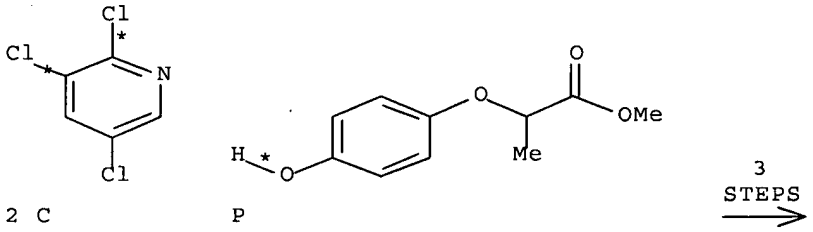
RX(6) RCT H 89402-43-7, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

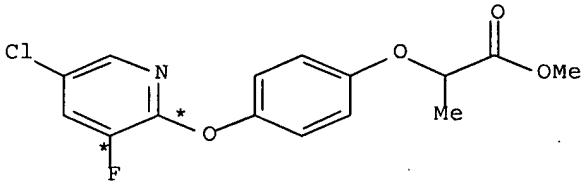
STAGE(2)
SOL 7732-18-5 Water

PRO O 105511-94-2

RX(37) OF 44 COMPOSED OF RX(2), RX(3), RX(9)
RX(37) 2 C + P ===> R



2 C P



R
YIELD 80%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

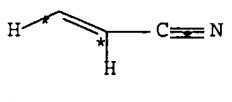
RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

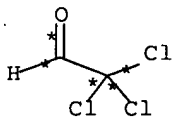
STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

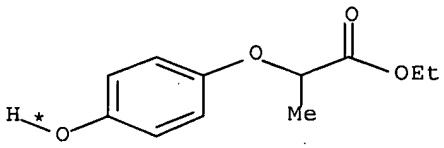
RX(38) OF 44 COMPOSED OF RX(1), RX(2), RX(3), RX(6)
RX(38) A + B + L ===> O



A

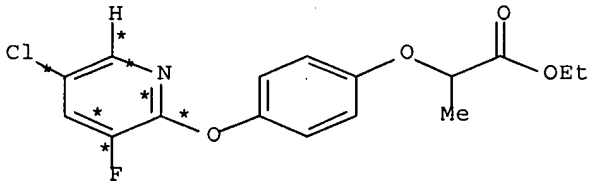


B



L

4 STEPS



O
YIELD 81%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7

SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

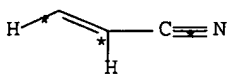
RX(6) RCT H 89402-43-7, L 65343-67-1

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

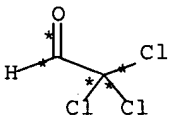
STAGE(2)
SOL 7732-18-5 Water

PRO O 105511-94-2

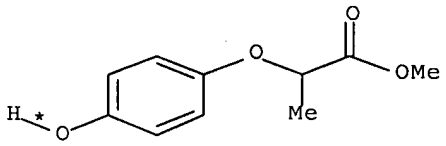
RX(39) OF 44 COMPOSED OF RX(1), RX(2), RX(3), RX(9)
RX(39) A + B + P ===> R



A

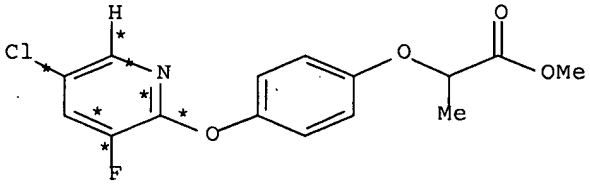


B



P

4 STEPS



R
YIELD 80%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(3) RCT G 823-56-3

RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

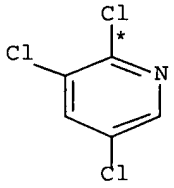
RX(9) RCT H 89402-43-7, P **60075-04-9**

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

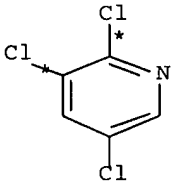
STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

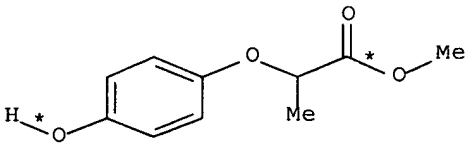
RX(40) OF 44 COMPOSED OF RX(2), RX(9), RX(15)
RX(40) 2 C + **P** ===> **AA**



C

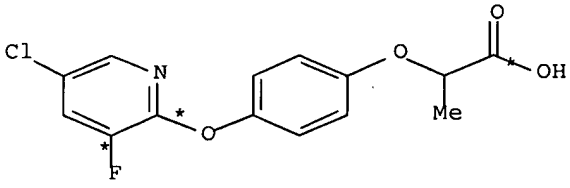


C



P

3
STEPS



AA
YIELD 82%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)

CON 10 hours, 200 deg C

RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

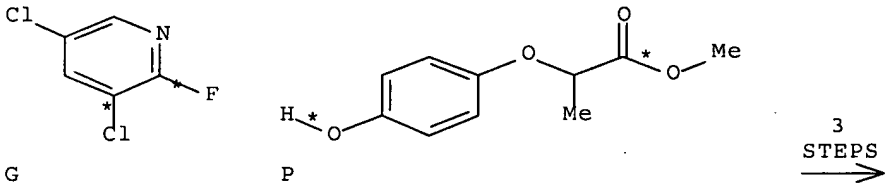
RX(15) RCT R 87035-49-2

STAGE(1)
RGT AB 1310-73-2 NaOH
SOL 123-91-1 Dioxane
CON 3 hours, 35 deg C

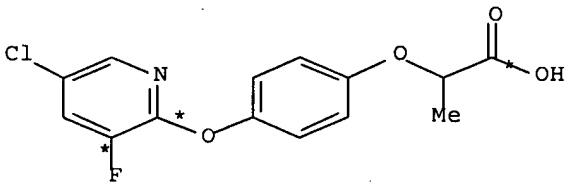
STAGE(2)
RGT AC 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AA 87135-08-8

RX(41) OF 44 COMPOSED OF RX(3), RX(9), RX(15)
RX(41) G + **P** ===> **AA**



G P



AA
YIELD 82%

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-,

tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

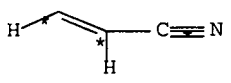
RX(15) RCT R 87035-49-2

STAGE(1)
RGT AB 1310-73-2 NaOH
SOL 123-91-1 Dioxane
CON 3 hours, 35 deg C

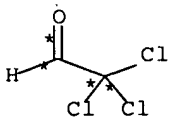
STAGE(2)
RGT AC 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AA 87135-08-8

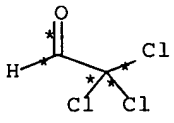
RX(42) OF 44 COMPOSED OF RX(1), RX(2), RX(9), RX(15)
RX(42) 2 A + 2 B + **P** ===> **AA**



2 A



B



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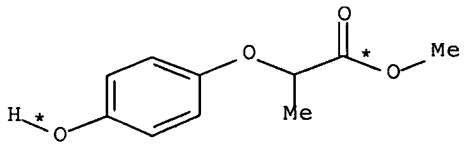
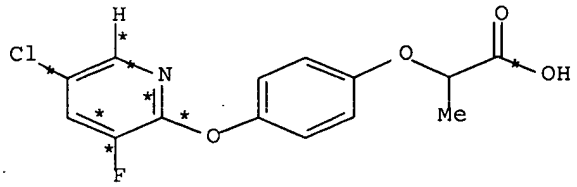


P

4
STEPS



AA
YIELD 82%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

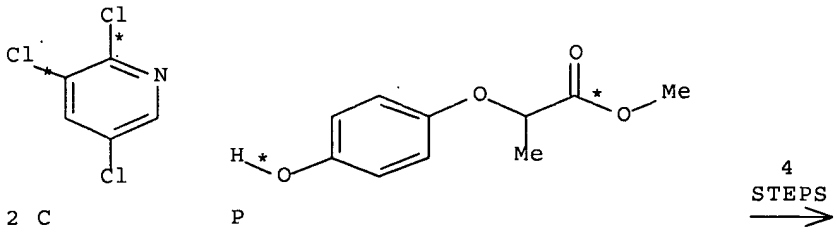
RX(15) RCT R 87035-49-2

STAGE(1)
RGT AB 1310-73-2 NaOH
SOL 123-91-1 Dioxane
CON 3 hours, 35 deg C

STAGE(2)
RGT AC 7647-01-0 HCl
SOL 7732-18-5 Water

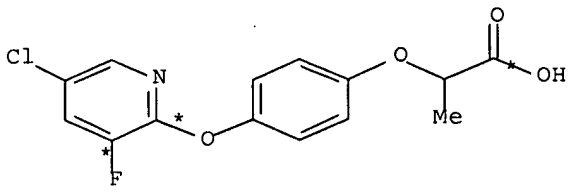
PRO AA 87135-08-8

RX(43) OF 44 COMPOSED OF RX(2), RX(3), RX(9), RX(15)
RX(43) 2 C + P ===> AA



2 C P

4 STEPS



AA
YIELD 82%

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(3) RCT G 823-56-3
RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

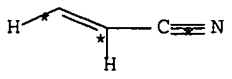
RX(15) RCT R 87035-49-2

STAGE(1)
RGT AB 1310-73-2 NaOH
SOL 123-91-1 Dioxane
CON 3 hours, 35 deg C

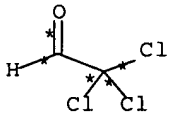
STAGE(2)
RGT AC 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AA 87135-08-8

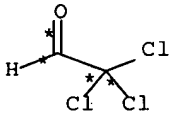
RX(44) OF 44 COMPOSED OF RX(1), RX(2), RX(3), RX(9), RX(15)
RX(44) 2 A + 2 B + P ===> **AA**



2 A



B



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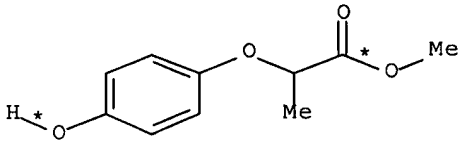
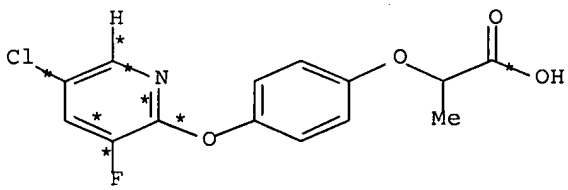


P

5
STEPS



AA
YIELD 82%

RX(1) RCT A 107-13-1, B 75-87-6
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
PRO C 16063-70-0
CAT 7758-89-6 CuCl
SOL 75-05-8 MeCN
CON 120 deg C

RX(2) RCT C 16063-70-0
RGT I 584-08-7 K2CO3, J 7789-23-3 KF, K 13400-13-0 CsF
PRO G 823-56-3, H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 10 hours, 200 deg C

RX(3) RCT G 823-56-3

RGT I 584-08-7 K2CO3, K 13400-13-0 CsF
PRO H 89402-43-7
SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-)
CON 8 hours, 100 - 110 deg C, 200 mmHg

RX(9) RCT H 89402-43-7, P 60075-04-9

STAGE(1)
RGT D 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-), I 584-08-7 K2CO3
SOL 75-05-8 MeCN
CON 40 hours, 50 - 60 deg C

STAGE(2)
SOL 7732-18-5 Water

PRO R 87035-49-2

RX(15) RCT R 87035-49-2

STAGE(1)
RGT AB 1310-73-2 NaOH
SOL 123-91-1 Dioxane
CON 3 hours, 35 deg C

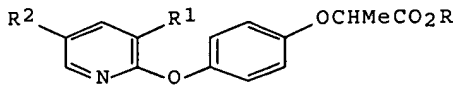
STAGE(2)
RGT AC 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AA 87135-08-8

L48 ANSWER 4 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 116:6426 CASREACT Full-text
TITLE: Solvent-free process for the preparation of [(pyridinyloxy)phenoxy]propionate derivatives
INVENTOR(S): Love, Jim; Grant, Charles B.; Gatling, Sterling
PATENT ASSIGNEE(S): DowElanco, USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5049675	A	19910917	US 1990-471347	19900129
EP 439857	A2	19910807	EP 1990-203426	19901219
EP 439857	A3	19911121		
EP 439857	B1	19941221		
R: CH, DE, ES, FR, GB, IT, LI, NL				
BR 9008621	A	19911119	BR 1990-8621	19901219
ES 2065473	T3	19950216	ES 1990-203426	19901219
AU 9169993	A	19910801	AU 1991-69993	19910125
JP 07070071	A	19950314	JP 1991-23738	19910125
HU 56067	A2	19910729	HU 1991-291	19910128
CA 2035107	A1	19910730	CA 1991-2035107	19910128
IL 97077	A	19950315	IL 1991-97077	19910128

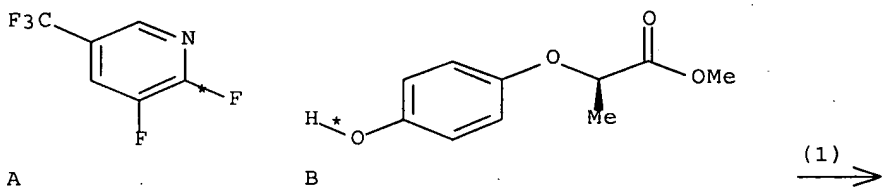
PRIORITY APPLN. INFO.: US 1990-471347 19900129
OTHER SOURCE(S): MARPAT 116:6426
GI



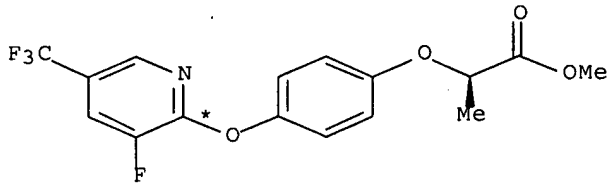
I

AB Phenoxypropionates I (R = alkyl; R1 = H, F, Cl; R2 = Cl, Br, iodo, CF3) were prepared by treating a 2-fluoropyridine with 4-HOC6H4OCHMeCO2R in the presence of an anhydrous base in the absence of solvent. Thus (R)-I (R = Me, R1 = F, R2 = CF3) was obtained in 96% yield and 99.2% purity from 2,3-difluoro-5-trifluoromethylpyridine and (R)-4-HOC6H4OCHMeCO2Me in the presence of K2CO3.

RX(1) OF 1 A + B ===> C



A B (1)

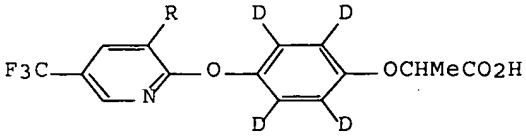


C
YIELD 96%

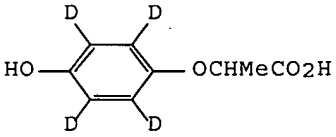
RX(1) RCT A 89402-42-6, B 96562-58-2
RGT D 584-08-7 K2CO3
PRO C 89402-39-1

L48 ANSWER 5 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 113:23634 CASREACT Full-text
TITLE: Synthesis of deuterium labelled analogs of fluazifop and haloxyfop
AUTHOR(S): Bartels, Michael J.; Gatling, Sterling C.
CORPORATE SOURCE: Dow Chem. Co., Midland, MI, 48674, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1990), 28(2), 235-40

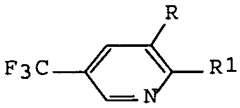
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



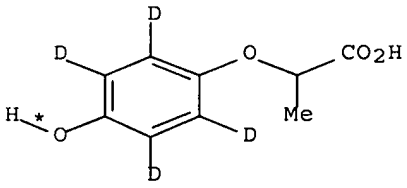
II



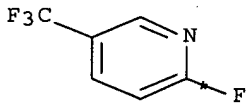
III

AB Title compds. I (R = H, Cl) were prepared by the condensation of phenoxypropanoic acid derivative II with pyridine derivs. III (R = H, R1 = F; R = R1 = Cl) resp. II was prepared via acid-catalyzed deuteration of 4-HOC6H4OCHMeCO2H.

RX(1) OF 2 **A** + **B** ===> **C**

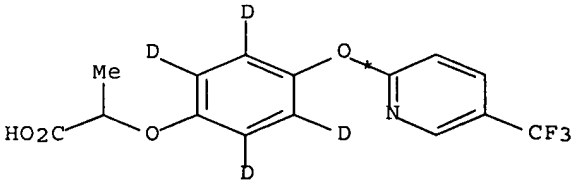


A



B

(1)



C
YIELD 82%

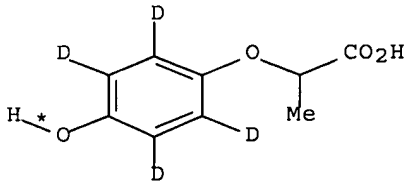
RX(1) RCT A 127893-32-7

STAGE(1)
RGT D 1310-73-2 NaOH
SOL 67-68-5 DMSO, 7732-18-5 Water

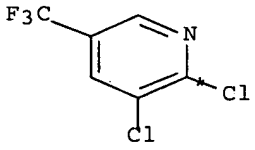
STAGE(2)
RCT B 69045-82-5

PRO C 127893-33-8

RX(2) OF 2 A + G ===> H

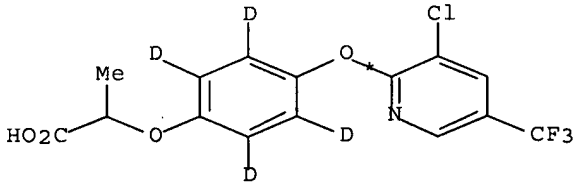


A



G

(2) →



H
YIELD 32%

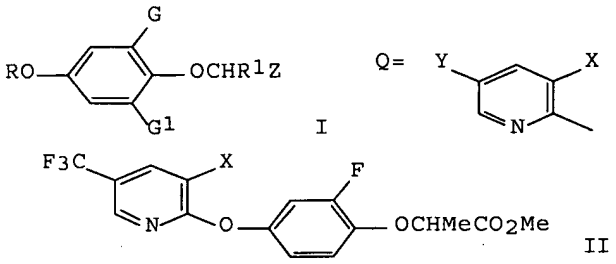
RX(2) RCT A 127893-32-7, G 69045-84-7
RGT I 584-08-7 K2CO3, J 4368-51-8 1-Heptanaminium, N,N,N-triheptyl-, bromide
PRO H 127893-34-9
SOL 127-18-4 Perchloroethene, 7732-18-5 Water

L48 ANSWER 6 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 111:57539 CASREACT Full-text
TITLE: Preparation of 2-[4-(3,5-disubstituted-2-pyridyloxy)fluorophenoxy]alkanoates as herbicides
INVENTOR(S): Rogers, Richard B.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 19 pp. Cont.-in-part of U.S. Ser. No. 550,328, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4750931	A	19880614	US 1985-787824	19851015
ZA 8408416	A	19860625	ZA 1984-8416	19841029
AU 8434896	A	19850516	AU 1984-34896	19841101
AU 576332	B2	19880825		
DK 8405351	A	19850511	DK 1984-5351	19841109
JP 60116649	A	19850624	JP 1984-236565	19841109
JP 02014342	B	19900406		
BR 8405719	A	19850910	BR 1984-5719	19841109
CA 1219585	A1	19870324	CA 1984-467435	19841109
US 4888050	A	19891219	US 1988-154821	19880211
PRIORITY APPLN. INFO.:			US 1983-550328	19831110
			US 1985-787824	19851015

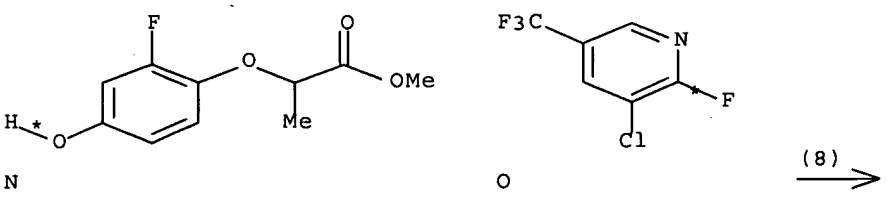
OTHER SOURCE(S): MARPAT 111:57539

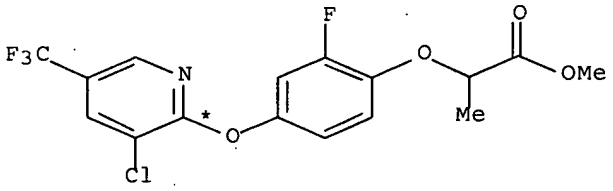
GI



AB The title compds. [I; 1 of G, G1 = F, the other = H, F; R = (un)substituted aryl, heteroaryl; R1 = C1-3 alkyl; Z = organic moiety containing N, O, or S atoms or a metallic, ammonium, or organic amine cation and is, or can be, hydrolyzed and/or oxidized in plants or soil to a carboxyl moiety in (un)dissociated form] were prepared 2,4-F(O2N)C6H3OH (preparation given) was stirred 45 min. at 100° with MeCHBrCO2Me in DMSO containing K2CO3 to give 2,4-F(O2N)C6H3OCHMeCO2Me which was reduced to the amine. The latter was diazotized and hydrolyzed to give 2,4-F(HO)C6H3OCHMeCO2Me which was stirred 30 min at 125-140° with chloropyridine QCl (X = Cl, Y = CF3) in DMSO containing K2CO3 to give title compound II (X = Cl) (III). Preemergence, 0.28 kg III/ha gave 100% control of barnyardgrass, yellow foxtail, Johnson grass and wild oats. III gave 100% postemergence control of crabgrass and the above weeds at 7.8-31.25 ppm.

RX(8) OF 34 **N** + O ===> **P**...

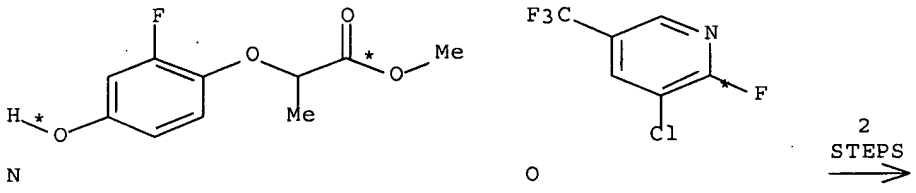




P
YIELD 87%

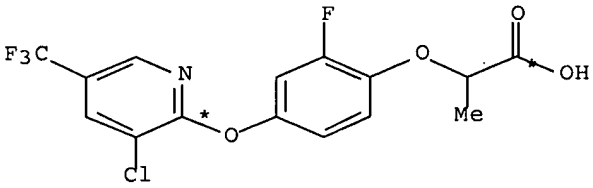
RX(8) RCT N 99045-15-5, O 72537-17-8
PRO P 99044-99-2

RX(25) OF 34 COMPOSED OF RX(8), RX(9)
RX(25) N + O ===> Q



N O

2 STEPS



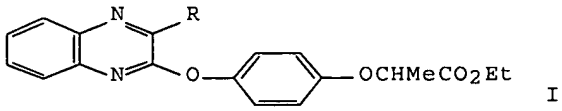
Q
YIELD 93%

RX(8) RCT N 99045-15-5, O 72537-17-8
PRO P 99044-99-2

RX(9) RCT P 99044-99-2
PRO Q 120594-32-3

L48 ANSWER 7 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 108:150426 CASREACT Full-text
TITLE: Synthesis of ethyl 2-[4-(3-fluoro-2-quinoxalinyloxy)phenoxy]propanoate as herbicide
AUTHOR(S): Makino, Kenzi; Yoshioka, Hirosuke
CORPORATE SOURCE: Inst. Phys. Chem. Res., Wako, 351-01, Japan

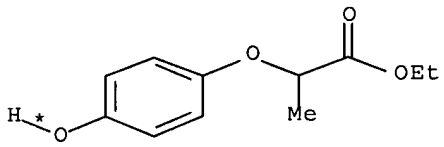
SOURCE: Journal of Fluorine Chemistry (1987), 37(1), 119-24
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



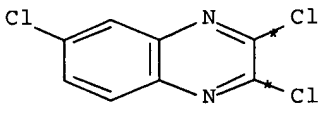
I

AB The syntheses of title compound I (R = F), a new fluoro analog of the herbicide quizalofopethyl, from 2,3-dichloroquinoxaline and of Et 2-[4-(6-chloro-3,4-dihydro-3-oxoquinoxalinyl-2-oxy)phenoxy]propanoate from Et 2-[4-(3,6-dichloro-2-quinoxalinyloxy)phenoxy]propanoate via nucleophilic substitution with CsF coupled with 18-crown-6 are described. The growth inhibitory activity of I (R = H, F, Cl, Me) on rice plants was examined The herbicidal activity of I increases in the decreasing order of bulkiness of R.

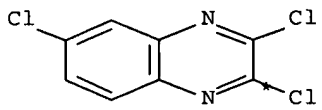
RX(6) OF 11 3 **F** + 2 K ===> **L** + M...



3 F

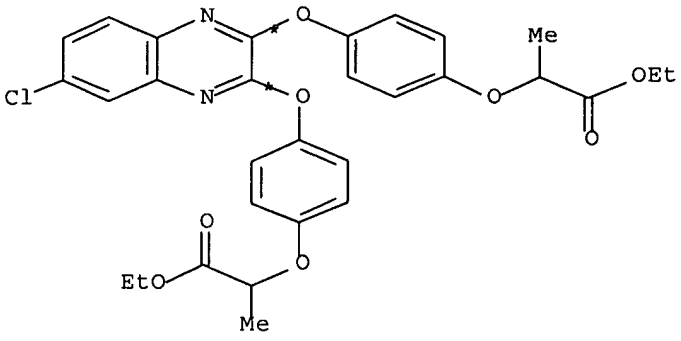


K

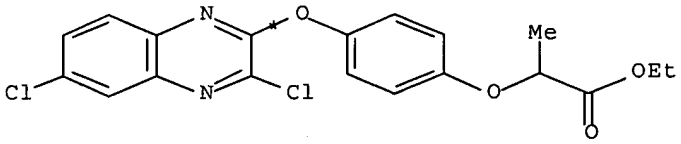


K

(6) →



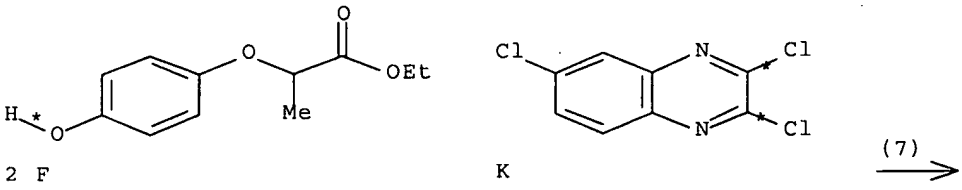
L



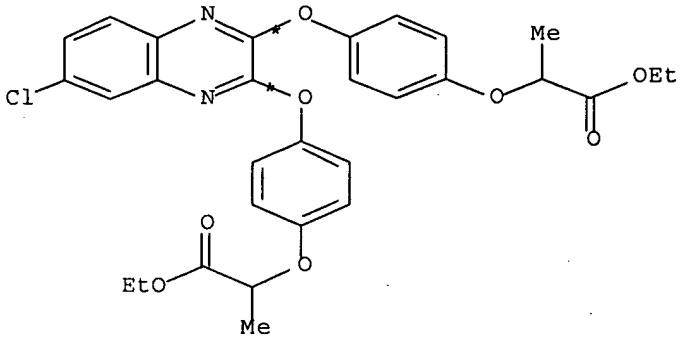
M

RX(6) RCT F 65343-67-1, K 2958-87-4
RGT H 584-08-7 K2CO3
PRO L 113760-13-7, M 113760-15-9
SOL 75-05-8 MeCN

RX(7) OF 11 2 F + K ===> L



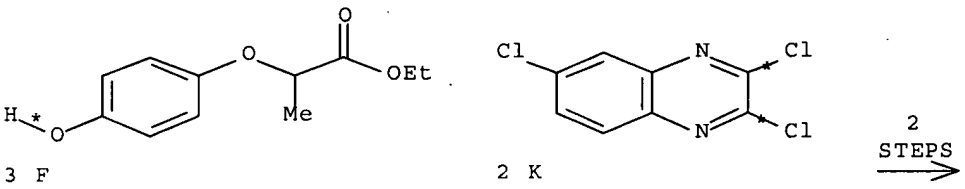
2 F K



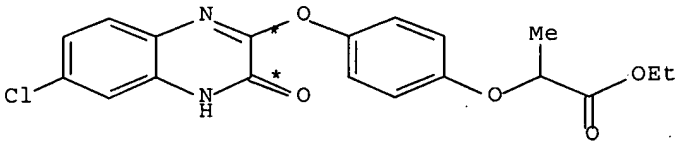
L
YIELD 29%

RX(7) RCT F 65343-67-1, K 2958-87-4
RGT C 13400-13-0 CsF, D 17455-13-9 18-Crown-6
PRO L 113760-13-7
SOL 109-99-9 THF

RX(11) OF 11 COMPOSED OF RX(6), RX(8)
RX(11) 3 F + 2 K ===> N



3 F 2 K 2 STEPS



N
YIELD 77%

RX(6) RCT F 65343-67-1, K 2958-87-4
RGT H 584-08-7 K2CO3
PRO L 113760-13-7, M 113760-15-9
SOL 75-05-8 MeCN

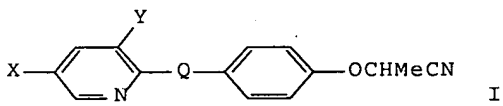
RX(8) RCT M 113760-15-9
RGT C 13400-13-0 CsF, D 17455-13-9 18-Crown-6
PRO N 113760-14-8
SOL 109-99-9 THF

L48 ANSWER 8 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 102:149124 CASREACT Full-text
TITLE: Herbicidal trifluoromethylpyridinyloxyphenoxy- and -pyridinylthiophenoxy propanenitriles and their derivatives
INVENTOR(S): Johnston, Howard; Troxell, Lillian H.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 16 pp. Division of U.S. Ser. No. 918,550.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4491468	A	19850101	US 1982-409811	19820820
US 4753673	A	19880628	US 1978-918550	19780623
EP 57473	A2	19820811	EP 1982-101502	19780630
EP 57473	A3	19830511		
R: BE, DE, FR, GB, NL, SE				
AU 8063039	A	19810205	AU 1980-63039	19801007
AU 529649	B2	19830616		
CA 1321590	C2	19930824	CA 1981-388668	19811023
US 4479001	A	19841023	US 1983-467552	19830217
AU 568503	B2	19880107	AU 1983-17941	19830812
AU 8317941	A	19831208		
US 4523017	A	19850611	US 1983-529178	19830902
US 4551170	A	19851105	US 1984-679976	19841210
US 4628099	A	19861209	US 1985-720844	19850408

PRIORITY APPLN. INFO.:
US 1977-817943 19770722
US 1978-918550 19780623
CA 1978-305900 19780621
AU 1978-37703 19780703
EP 1980-101361 19801029
US 1982-357346 19820311
US 1982-409791 19820820
US 1982-409811 19820820

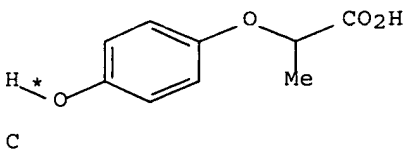
GI



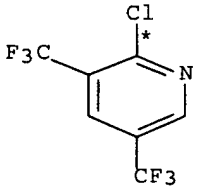
I

AB Several examples of the title compds. I (Q = O, S; X = Cl, Br, CF3; Y = H, Cl, Br, CF3, and at least one of X or Y is CF3) and their derivs., preemergent and postemergent herbicides, were prepared Thus, treating 2-(4-hydroxyphenoxy)propanoic acid with 2-chloro-3,5- bis(trifluoromethyl)pyridine in presence of NaOH gave 2-[4-[3,5- bis(trifluoromethyl)-2-pyridinyloxy]phenoxy]propanoic acid (II). II was also amidated, or reduced, then esterified to produce derivs. At 1 lb/acre, I (X = Cl, Y = CF3, Q = O) gave 100% control of Johnson grass.

RX(2) OF 26 C + D ===> E...

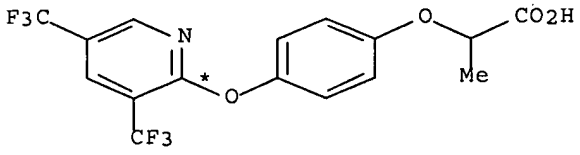


C



D

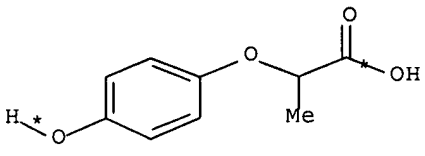
(2) →



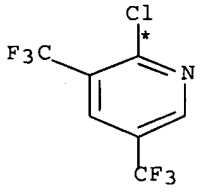
E

RX(2) RCT C 67648-61-7, D 70158-60-0
PRO E 70158-55-3

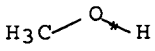
RX(12) OF 26 COMPOSED OF RX(2), RX(3)
RX(12) C + D + F ===> G



C

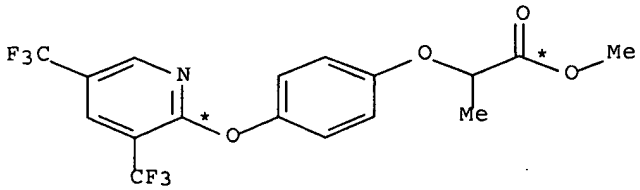


D



F

2 STEPS →



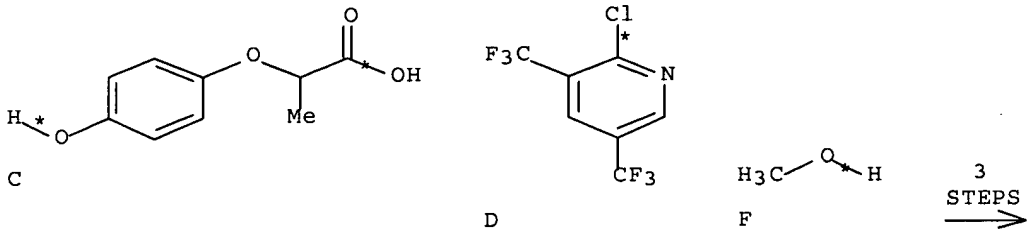
G

RX(2) RCT C 67648-61-7, D 70158-60-0

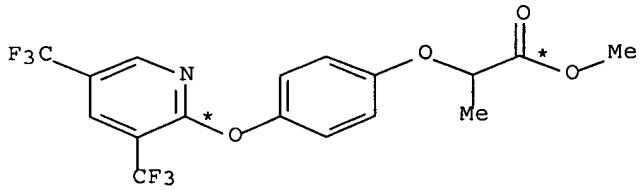
PRO E 70158-55-3

RX(3) RCT E 70158-55-3, F 67-56-1
PRO G 70158-66-6

RX(19) OF 26 COMPOSED OF RX(2), RX(11), RX(10)
RX(19) C + D + F ===> G



C D F



G

RX(2) RCT C 67648-61-7, D 70158-60-0
PRO E 70158-55-3

RX(11) RCT E 70158-55-3
RGT H 7719-09-7 SOCl2
PRO V 74900-19-9

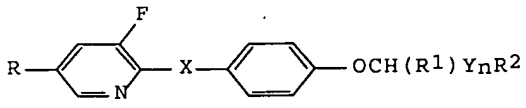
RX(10) RCT V 74900-19-9, F 67-56-1
PRO G 70158-66-6
CAT 121-44-8 Et3N

L48 ANSWER 9 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 103:191463 CASREACT Full-text
TITLE: Herbicide compositions containing pyridinyloxyphenoxyalkanoic acids, pyridinylthiophenoxyalkanoic acids, and their derivatives
INVENTOR(S): Johnson, Howard; Troxell, Lillian H.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: Ger. (East), 55 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 217694	A5	19850123	DD 1983-257404	19831201

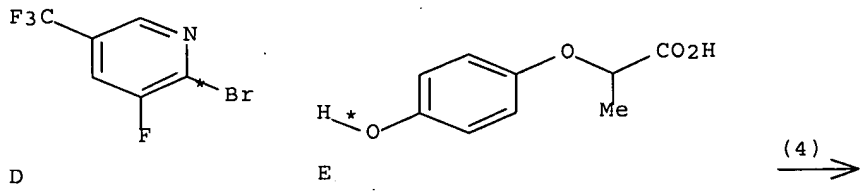
PRIORITY APPLN. INFO.: DD 1983-257404 19831201
GI



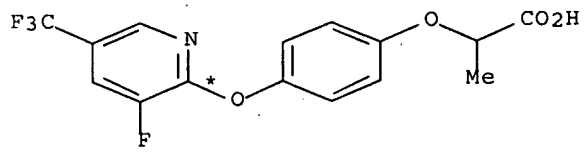
I

AB The title compds. I (R = CF3, CHF2, CClF2, Br; R1 = H, alkyl; R2 = CO2H; X = O, S; Y = alkylene; n = 0-1) are herbicides. Thus, in the greenhouse, 7.8 ppm Me 2-[4-(3-fluoro-5-chloro-2-pyridinyloxy)phenoxy]propionate [87035-49-2] totally controlled barnyard grass (Echinochloa crus-galli) and other weeds, with no phytotoxicity to soybean, cotton, and other culture plants. The preparation of I is given.

RX(4) OF 28 ...D + **E** ===> **F**...



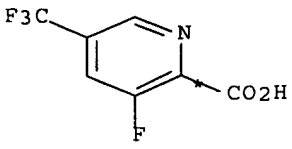
D E (4)



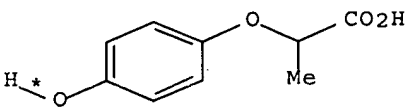
F

RX(4) RCT D 89402-29-9, E 67648-61-7
PRO F 89402-30-2

RX(10) OF 28 COMPOSED OF RX(3), RX(4)
RX(10) C + **E** ===> **F**

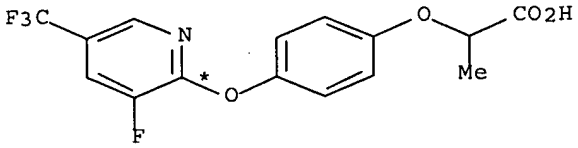


C



E

2 STEPS

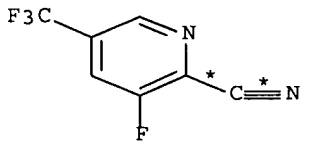


F

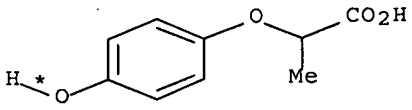
RX(3) RCT C 89402-28-8
PRO D 89402-29-9

RX(4) RCT D 89402-29-9, E 67648-61-7
PRO F 89402-30-2

RX(15) OF 28 COMPOSED OF RX(2), RX(3), RX(4)
RX(15) B + E ===> F

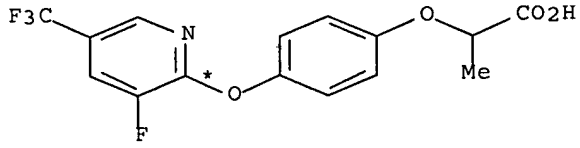


B



E

3 STEPS



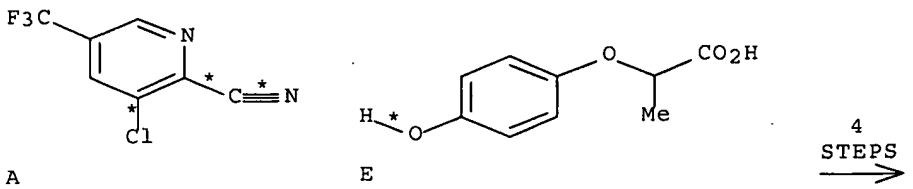
F

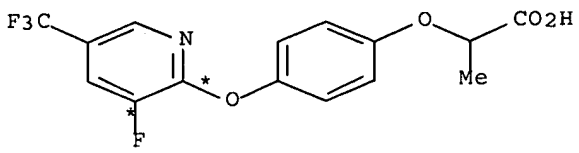
RX(2) RCT B 80194-71-4
PRO C 89402-28-8

RX(3) RCT C 89402-28-8
PRO D 89402-29-9

RX(4) RCT D 89402-29-9, E 67648-61-7
PRO F 89402-30-2

RX(16) OF 28 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(16) A + E ===> F





F

RX(1) RCT A 80194-70-3
PRO B 80194-71-4

RX(2) RCT B 80194-71-4
PRO C 89402-28-8

RX(3) RCT C 89402-28-8
PRO D 89402-29-9

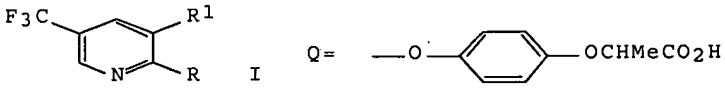
RX(4) RCT D 89402-29-9, E 67648-61-7
PRO F 89402-30-2

L48 ANSWER 10 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 101:72612 CASREACT Full-text
TITLE: 2,3-Difluoro-5-(trifluoromethyl)pyridine as intermediate for herbicides
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59020269	A	19840201	JP 1983-110035	19830618
JP 04046271	B	19920729		
US 4480102	A	19841030	US 1982-401057	19820723
EP 104715	A2	19840404	EP 1983-303323	19830608
EP 104715	A3	19841227		
EP 104715	B1	19881012		

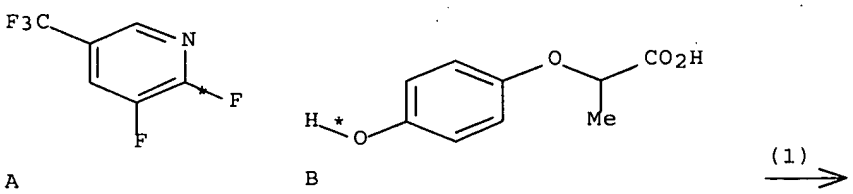
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
DK 8302812	A	19840124	DK 1983-2812	19830617
DK 160490	B	19910318		
DK 160490	C	19910826		
ZA 8304460	A	19850227	ZA 1983-4460	19830617
CA 1202308	A1	19860325	CA 1983-432386	19830713
HU 32349	A2	19840730	HU 1983-2596	19830722
HU 188479	B	19840730		
US 4625035	A	19861125	US 1985-789791	19851021
JP 05065272	A	19930319	JP 1992-54142	19920206
JP 07061997	B	19950705		
PRIORITY APPLN. INFO.:			US 1982-401057	19820723
			US 1984-621343	19840618

GI

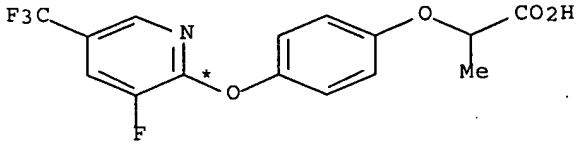


AB The title compound (I, R = R1 = F) (II), intermediate for herbicidal (no data) [(pyridyloxy)phenoxy]alkanoic acids, was prepared Thus, a mixture of 50 mL Me2SO, 1.9 g CsF, and about 0.5 g K2CO3 was heated at 115° until a yellowish solution resulted, the temperature lowered to 70°, 1.98 g I (R = F, R1 = Cl) added and the resulting mixture heated at 105° for 21 h to give II (yield not given). Treatment of II with HQ in Me2SO-H2O containing NaOH at 70-80° gave I (R = Q, R1 = F).

RX(1) OF 3 ...A + **B** ===> **C**



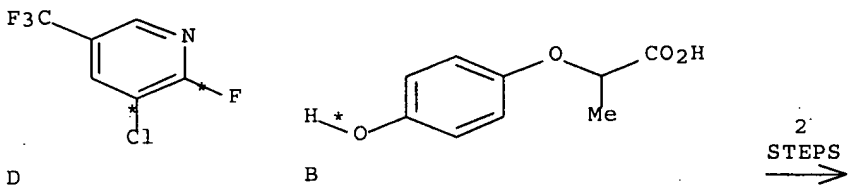
A B (1)



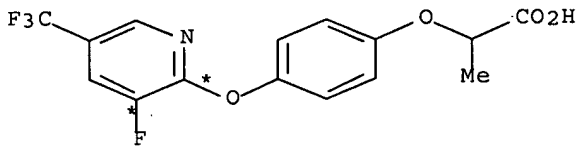
C

RX(1) RCT A 89402-42-6, B 67648-61-7
PRO C 89402-30-2

RX(3) OF 3 COMPOSED OF RX(2), RX(1)
RX(3) D + B ===> C



D B



C

RX(2) RCT D 72537-17-8
PRO A 89402-42-6

RX(1) RCT A 89402-42-6, B 67648-61-7
PRO C 89402-30-2

L48 ANSWER 11 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 100:138965 CASREACT Full-text
TITLE: Pyridyl(oxy/thio)phenoxy compounds and herbicidal compositions
INVENTOR(S): Johnston, Howard; Troxell, Lillian Heitz
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: Eur. Pat. Appl., 57 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 97460	A1	19840104	EP 1983-303353	19830609
EP 97460	B1	19880406		
R: AT, BE, CH, DE, FR, IT, LI, NL, SE				
US 4565568	A	19860121	US 1983-497295	19830523
IL 68822	A	19900712	IL 1983-68822	19830531
AU 8315334	A	19831215	AU 1983-15334	19830602
AU 556172	B2	19861023		
GB 2123819	A	19840208	GB 1983-15847	19830609
GB 2123819	B	19860416		

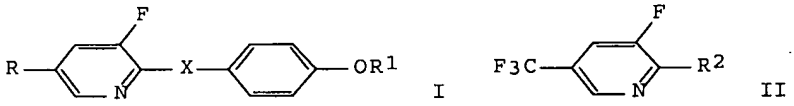
AT 33387	T	19880415	AT 1983-303353	19830609
DK 8302811	A	19831219	DK 1983-2811	19830617
DK 157015	B	19891030		
DK 157015	C	19900326		
BR 8303329	A	19840207	BR 1983-3329	19830617
ES 523398	A1	19841001	ES 1983-523398	19830617
CA 1179350	A1	19841211	CA 1983-430592	19830617
ZA 8304462	A	19850227	ZA 1983-4462	19830617
JP 59007165	A	19840114	JP 1983-110033	19830618
JP 62049269	B	19871019		
HU 36458	A2	19850930	HU 1983-3719	19831028
HU 189768	B	19860728		
ES 530713	A1	19850501	ES 1984-530713	19840316
ES 530712	A1	19850516	ES 1984-530712	19840316
CA 1182459	A2	19850212	CA 1984-457507	19840626
US 4678509	A	19870707	US 1985-793865	19851101
US 4851539	A	19890725	US 1985-799702	19851119
JP 62142156	A	19870625	JP 1986-275483	19861120
JP 62142154	A	19870625	JP 1986-275484	19861120
JP 62142157	A	19870625	JP 1986-275485	19861120
US 33478	E	19901211	US 1988-267490	19881031

PRIORITY APPLN. INFO.:

US 1982-389840 19820618
US 1983-497295 19830523
EP 1983-303353 19830609
CA 1983-430592 19830617

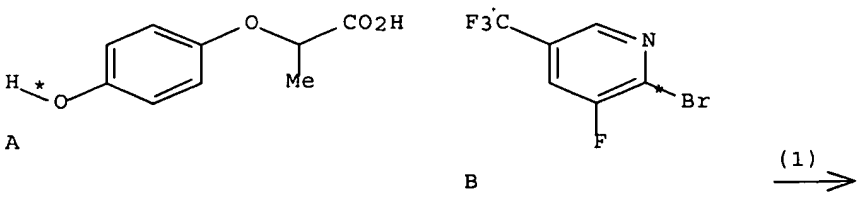
OTHER SOURCE(S): MARPAT 100:138965

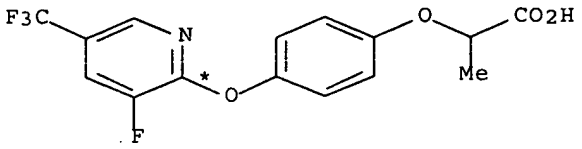
GI



AB The title compds. I (X = O, S; R = CF3, CHF2, CClF2, Br, Cl; R1 = hydrolyzable or oxidizable organic group) were prepared Thus, 3-chloro-2-fluoro-5-trifluoromethylpyridine was treated with KCN and the resulting nitrile was fluorinated to give II (R2 = cyano). Hydrolysis of the nitrile group and treatment of the acid with Br gave II (R2 = Br) which was treated with 4-HOC6H4OCHMeCO2H to give II (R2 = 4-OC6H4OCHMeCO2H) (III). At 31.25 ppm post-emergence III gave 100% control of e.g. barnyardgrass.

RX(1) OF 34 A + B ===> C...

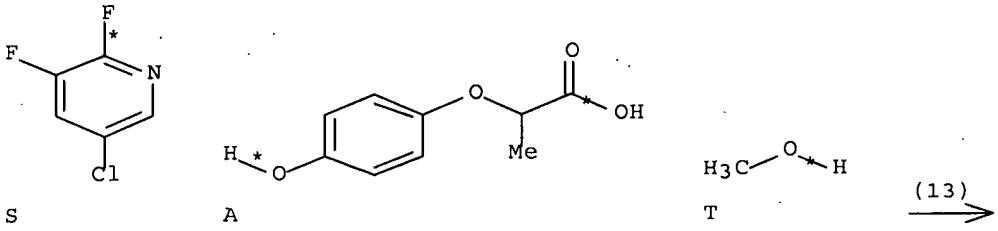




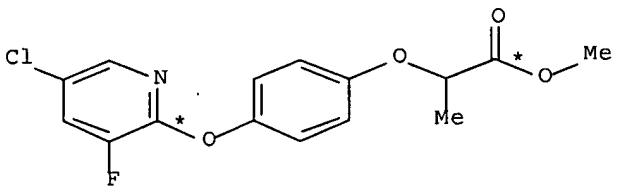
C

RX(1) RCT A 67648-61-7, B 89402-29-9
PRO C 89402-30-2

RX(13) OF 34 ...S + A + T ===> U



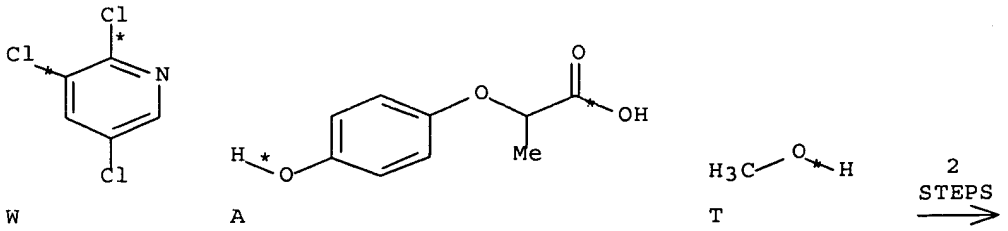
S A T (13)



U

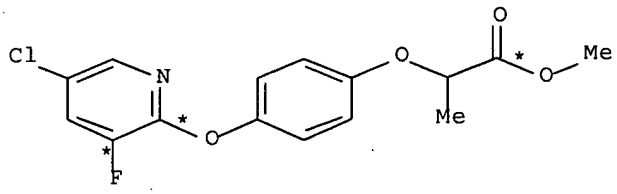
RX(13) RCT S 89402-43-7, A 67648-61-7, T 67-56-1
PRO U 87035-49-2

RX(25) OF 34 COMPOSED OF RX(15), RX(13)
RX(25) W + A + T ===> U



W A T

2 STEPS

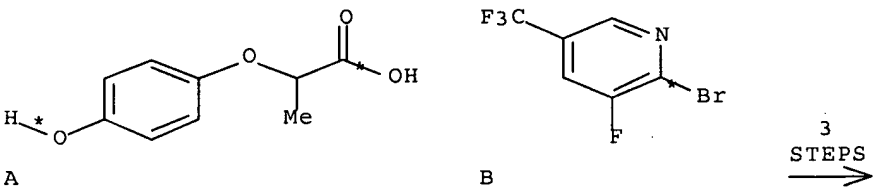


U

RX(15) RCT W 16063-70-0
PRO S 89402-43-7

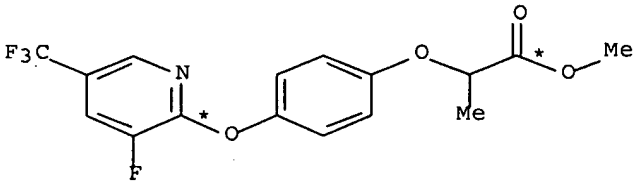
RX(13) RCT S 89402-43-7, A 67648-61-7, T 67-56-1
PRO U 87035-49-2

RX(28) OF 34 COMPOSED OF RX(1), RX(3), RX(6)
RX(28) A + B ===> I



A B

3 STEPS



I

RX(1) RCT A 67648-61-7, B 89402-29-9
PRO C 89402-30-2

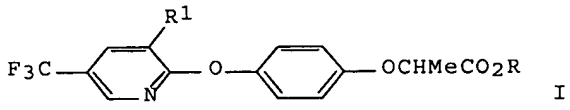
RX(3) RCT C 89402-30-2
PRO F 89402-33-5

RX(6) RCT F 89402-33-5
PRO I 89402-34-6

L48 ANSWER 12 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 97:23638 CASREACT Full-text
TITLE: Herbicidal and plant growth regulating pyridyloxyphenoxypropionic acid derivatives
INVENTOR(S): Rempfler, Hermann; Schurter, Rolf; Foery, Werner
PATENT ASSIGNEE(S): Ciba-Geigy Corp. , USA
SOURCE: U.S., 8 pp. Cont.-in-part of U.S. Ser. No. 860,409.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4325729	A	19820420	US 1980-206518	19801113
SU 1120916	A3	19841023	SU 1977-2558101	19771226
PRIORITY APPLN. INFO.:			US 1977-860409	19771213

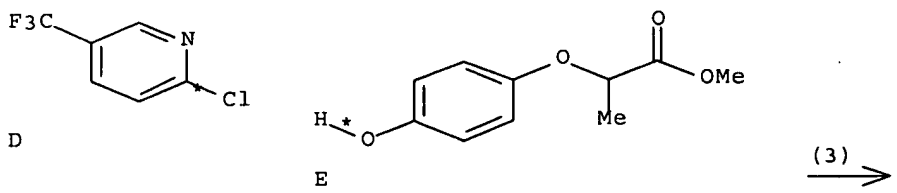
OTHER SOURCE(S): MARPAT 97:23638
GI

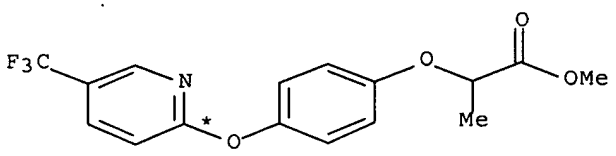


I

AB Esters I (R = cyanoalkyl, R1 = H or halo) were prepared, and they are useful as herbicides and plant growth regulators (no data). Thus, 4-HOC6H4OCHMeCO2Me in Me2SO was treated with NaH in Me2SO, the mixture was stirred, 2,6-dichloro-3-(trifluoromethyl)pyridine was introduced, and the new mixture was stirred 2 h to give I (R = Me, R1 = Cl). Also prepared was I (R = CH2CN, R1 = Cl).

RX(3) OF 7 D + E ===> A...

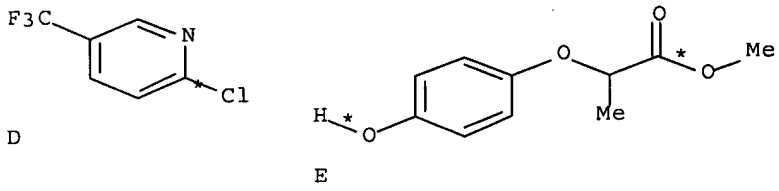




A

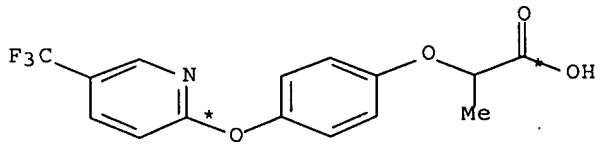
RX(3) RCT D 52334-81-3, E 60075-04-9
PRO A 69335-90-6

RX(6) OF 7 COMPOSED OF RX(3), RX(1)
RX(6) D + E ===> B



D E

2 STEPS

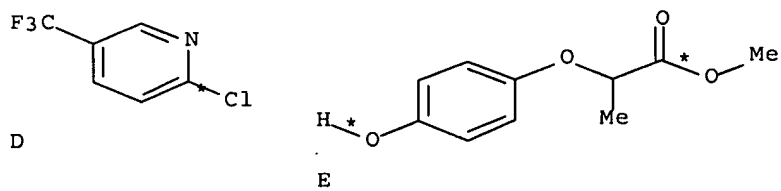


B

RX(3) RCT D 52334-81-3, E 60075-04-9
PRO A 69335-90-6

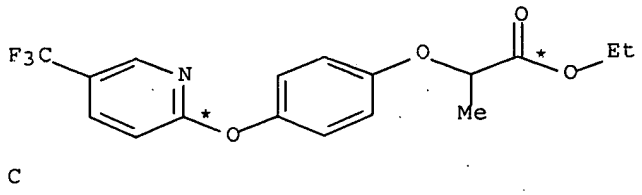
RX(1) RCT A 69335-90-6
PRO B 69335-91-7

RX(7) OF 7 COMPOSED OF RX(3), RX(1), RX(2)
RX(7) D + E ===> C



D E

3 STEPS



C

RX(3) RCT D 52334-81-3, E 60075-04-9
PRO A 69335-90-6

RX(1) RCT A 69335-90-6
PRO B 69335-91-7

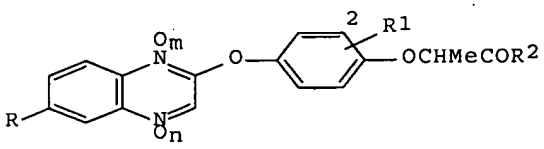
RX(2) RCT B 69335-91-7
PRO C 69045-80-3

L48 ANSWER 13 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 98:53933 CASREACT Full-text
TITLE: Quinoxaline derivatives as herbicides
PATENT ASSIGNEE(S): ICI Australia Ltd., Australia
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57140771	A	19820831	JP 1982-2384	19820112
JP 04074352	B	19921126		
AU 8179153	A	19820722	AU 1981-79153	19810112
AU 547454	B2	19851024		
US 4655819	A	19870407	US 1981-334384	19811224
IL 64707	A	19870831	IL 1982-64707	19820104
ZA 8200045	A	19821124	ZA 1982-45	19820105
EP 60607	A1	19820922	EP 1982-300074	19820107
EP 60607	B1	19850828		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AT 15192	T	19850915	AT 1982-300074	19820107
BR 8200079	A	19821116	BR 1982-79	19820108
HU 28591	A2	19831228	HU 1982-48	19820108
HU 186463	B	19850828		
ES 508629	A1	19821101	ES 1982-508629	19820111
CS 228911	B2	19840514	CS 1982-211	19820111
CA 1212676	A1	19861014	CA 1982-393929	19820112
US 4803273	A	19890207	US 1986-939694	19861209
PRIORITY APPLN. INFO.:			AU 1981-7201	19810112
			AU 1979-9617	19790717
			AU 1980-3093	19800411
			US 1980-164933	19800701
			US 1981-334384	19811224
			EP 1982-300074	19820107

OTHER SOURCE(S): MARPAT 98:53933

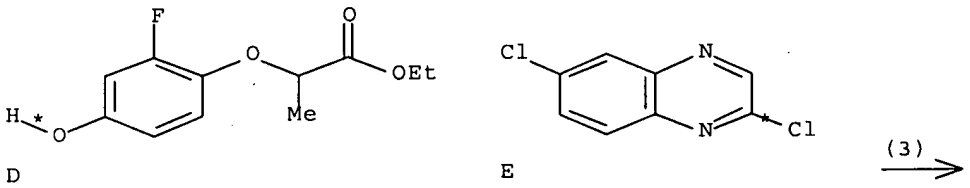
GI



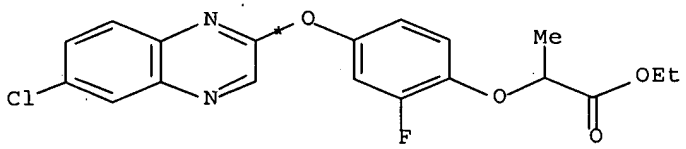
I

AB Seventeen quinoxaline derivs. (I; R,R1 = halo, Me, halomethyl; R2 = HO, HS, C1-10 alkoxy, C2-10 alkenloxy, cycloalkoxy, etc.; m, n = 0.1), effective herbicides at 0.25-5.0 kg/ha, were prepared Thus, a mixture of 2-fluoro-4-benzyloxyphenol 0.054, Et 2-bromopropionate 0.054, and K2CO3 0.059 mol in MeCOEt was refluxed 3 h to give 75% 2,4- F(PhCH2O)C6H3OCHMeCO2Et, which was treated with atmospheric H over 10% Pd-C to give 95% 2,4-F(HO)C6H3OCHMeCO2Et, which (0.005 mol) was heated with 0.005 mol 2,6-dichloroquinoxaline and 0.0055 mol K2CO2 in DMF at 100° to give 66% I (R = Cl, R1 = 2-F, R2 = EtO, m = n = 0).

RX(3) OF 17 ...D + E ===> F...



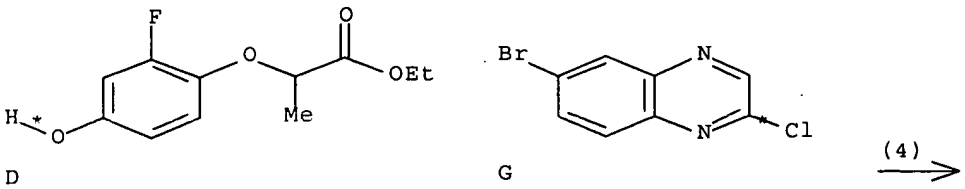
D E (3)



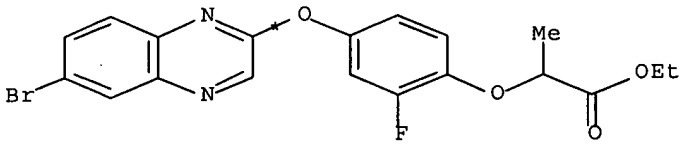
F

RX(3) RCT D 78689-30-2, E 18671-97-1
PRO F 84352-12-5

RX(4) OF 17 ...D + G ===> H...



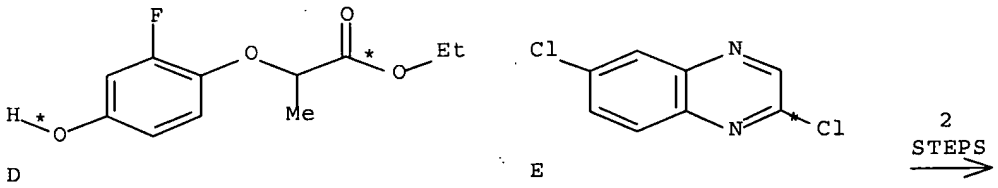
D G (4)



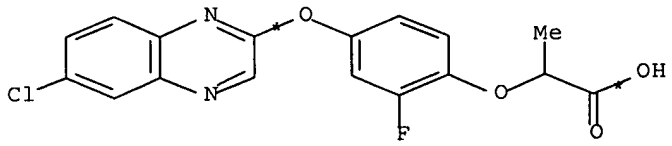
H

RX(4) RCT D 78689-30-2, G 55687-02-0
PRO H 84352-21-6

RX(10) OF 17 COMPOSED OF RX(3), RX(5)
RX(10) D + E ===> I



D E 2 STEPS

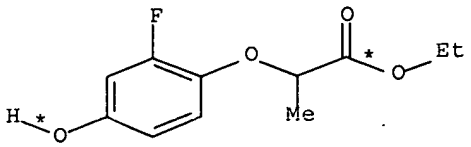


I

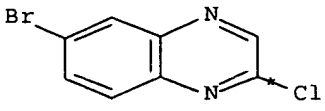
RX(3) RCT D 78689-30-2, E 18671-97-1
PRO F 84352-12-5

RX(5) RCT F 84352-12-5
PRO I 84352-20-5

RX(11) OF 17 COMPOSED OF RX(4), RX(6)
RX(11) D + G ===> J

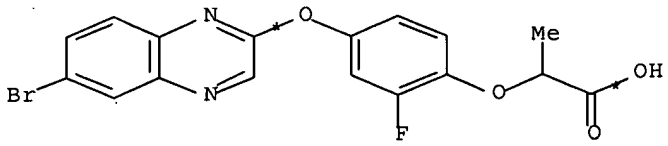


D



G

2 STEPS



J

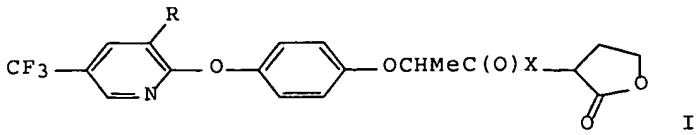
RX(4) RCT D 78689-30-2, G 55687-02-0
PRO H 84352-21-6

RX(6) RCT H 84352-21-6
PRO J 84352-24-9

L48 ANSWER 14 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 97:182223 CASREACT Full-text
TITLE: α-[(5'-Trifluoromethylpyridyl-2'-oxy)phenoxy]propionic acid γ-butyrolactone ester and thioester with a herbicidal effects, their production and applications
INVENTOR(S): Boehner, Beat; Rempfler, Hermann
PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3131363	A1	19820826	DE 1981-3131363	19810807
CH 645375	A5	19840928	CH 1980-6060	19800811
US 4395277	A	19830726	US 1981-288860	19810731
PRIORITY APPLN. INFO.:			CH 1980-6060	19800811

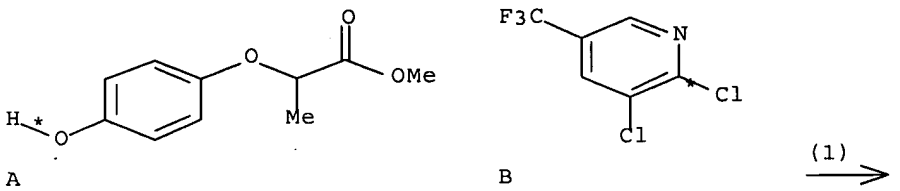
GI



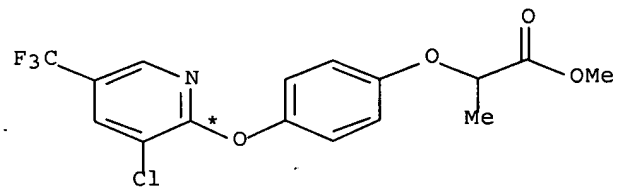
I

AB I (R = H, Cl; X = O, S) were prepared and shown to be active as herbicides. Thus, 4-HOC6H4OCHMeCO2Me was etherified with 2,3-dichloro-5-(trifluoromethyl)pyridine, saponified, and treated with α-bromo-γ-butyrolactone to give I (R = Cl, X = O).

RX(1) OF 2 A + B ===> C



A B



C

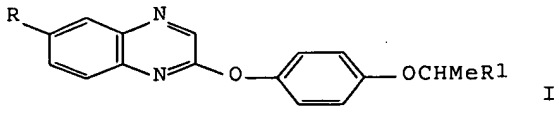
RX(1) RCT A 60075-04-9, B 69045-84-7
PRO C 69806-40-2

L48 ANSWER 15 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 96:6755 CASREACT Full-text
TITLE: Herbicidal quinoxalines
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 56057769	A	19810520	JP 1979-132819	19791017
PRIORITY APPLN. INFO.:			JP 1979-132819	19791017

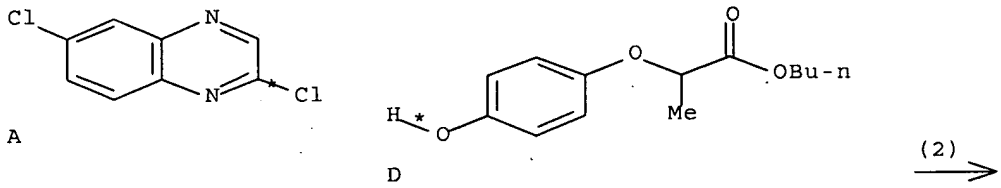
GI



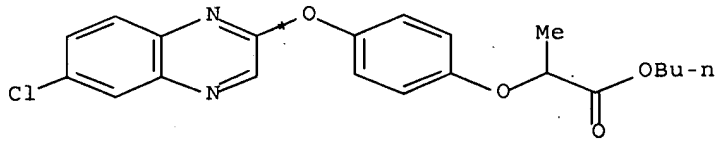
I

AB Twenty-six herbicidal quinoxalines I (R = Cl, F; R1 = CO2Bu, CONMe2, CO2Na, CH2OH, CH:CHCO2Me, etc.) were prepared via various routes. I caused no damage to cotton or soybean at 5-10 kg/ha by foliar application. Thus, 2,6-dichloroquinoxaline 10 was heated with p-HOC6H4OCHMeCO2Pr 10 and K2CO3 14 mmol in MeCN 12 h to give 86% I (R = Cl, R1 = CO2Pr).

RX(2) OF 24 A + D ===> E



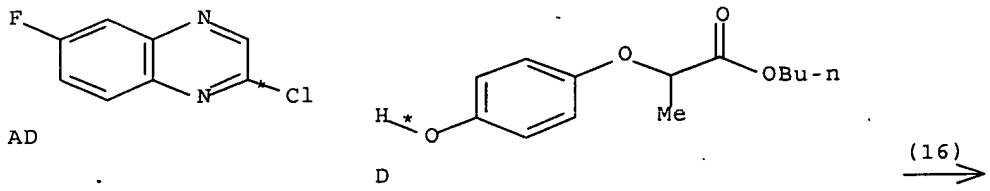
A D (2)



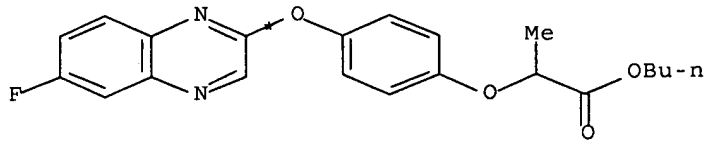
E

RX(2) RCT A 18671-97-1, D 81947-94-6
PRO E 76578-39-7

RX(16) OF 24 AD + D ===> AF



AD D



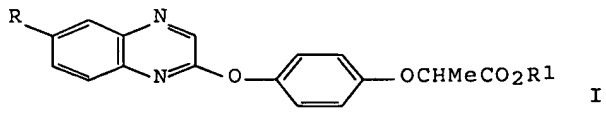
AF

RX(16) RCT AD 55687-33-7, D 81947-94-6
PRO AF 76578-52-4

L48 ANSWER 16 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 95:115603 CASREACT Full-text
TITLE: Quinoxaline derivatives
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56046868	A	19810428	JP 1979-124466	19790927

PRIORITY APPLN. INFO.: JP 1979-124466 19790927
GI

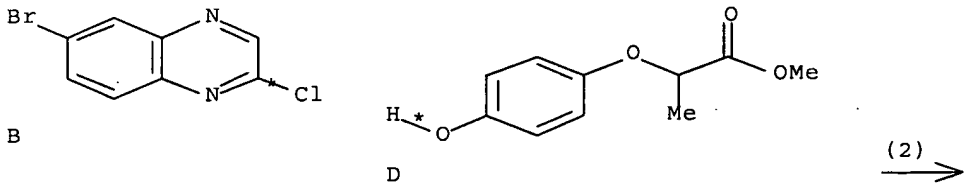


I

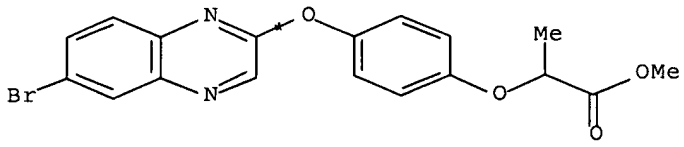
AB Quinoxaline derivs. I (R, R1 = Br, H; Br, Me; Br, Et; Br, Me2CH; iodo, Me; Me, Me; Me, Et; Me, Me2CH; Br, Na) were prepared and used as herbicides (data given against Echinochloa crus-galli, Digitaria adscendens, Portulaca oleracea, etc.). Thus, 56.1 g 3,4-(H2N)2C6H3Br in H2O was added to an aqueous mixture of 32.1 g NaIO4 and 39.3 g di-Bu L-(+)-tartrate and the whole stirred 3 h at 70-80° to give 65% 2-hydroxy-6- bromoquinoxaline, which (22.5 g) was refluxed with POCl3 2 h to give 83% 2-chloro-6-bromoquinoxaline, which (2.4 g) was refluxed with 2.4 g 4-HOC6H4OCHMeCO2Me and 2 g K2CO3 in MeCN 12 h to give

67% I (R = Br, R1 = Me) (II). Hydrolysis of II with aqueous NaOH by refluxing 1 h gave 84% I (R = Br, R1 = H).

RX(2) OF 3 ...B + D ===> E



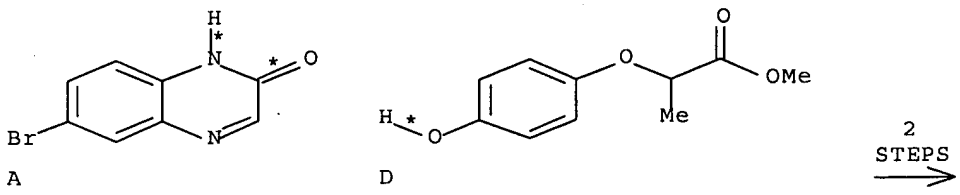
B D (2)



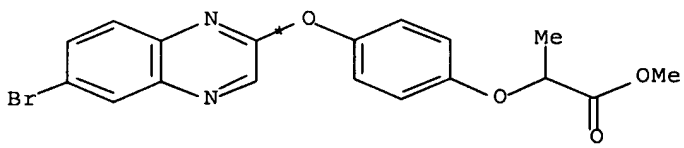
E

RX(2) RCT B 55687-02-0, D 60075-04-9
PRO E 76578-33-1
CAT 584-08-7 K2CO3

RX(3) OF 3 COMPOSED OF RX(1), RX(2)
RX(3) A + D ===> E



A D 2 STEPS



E

RX(1) RCT A 55687-34-8

RGT C 10025-87-3 POCl3
PRO B 55687-02-0

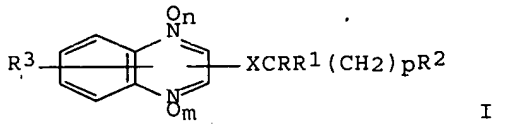
RX(2) RCT B 55687-02-0, D 60075-04-9
PRO E 76578-33-1
CAT 584-08-7 K2CO3

L48 ANSWER 17 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 95:25134 CASREACT Full-text
TITLE: Quinoxalinyloxyphenoxyalkane carboxylic acid derivatives and their use as herbicides
INVENTOR(S): Serban, Alexander; Watson, Keith Geoffrey; Farquharson
PATENT ASSIGNEE(S): ICI Australia Ltd., Australia
SOURCE: Eur. Pat. Appl., 63 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

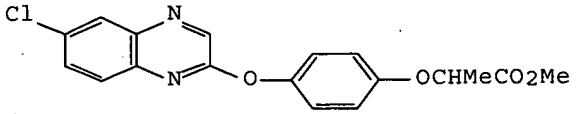
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 23785	A2	19810211	EP 1980-302411	19800717
EP 23785	A3	19810429		
EP 23785	B1	19850403		
R: AT, BE, CH, DE, FR, GB, IT, NL, SE				
AU 540234	B2	19841108	AU 1980-59547	19790717
AU 8059547	A	19810806		
ZA 8003928	A	19810624	ZA 1980-3928	19800630
IL 60506	A	19861231	IL 1980-60506	19800706
CA 1314549	C	19930316	CA 1980-356027	19800711
HU 26554	A2	19830928	HU 1980-1762	19800715
HU 186299	B	19850729		
DK 8003068	A	19810118	DK 1980-3068	19800716
DK 160426	B	19910311		
DK 160426	C	19910819		
BR 8004413	A	19810127	BR 1980-4413	19800716
ES 493431	A1	19810701	ES 1980-493431	19800716
CS 239908	B2	19860116	CS 1980-5044	19800716
SU 1261564	A1	19860930	SU 1980-2951003	19800716
JP 56039077	A	19810414	JP 1980-96960	19800717
JP 06013489	B	19940223		
AT 12495	T	19850415	AT 1980-302411	19800717
US 4655819	A	19870407	US 1981-334384	19811224
US 4803273	A	19890207	US 1986-939694	19861209
DK 8901684	A	19890407	DK 1989-1684	19890407
DK 168380	B1	19940321		
DK 8901685	A	19890407	DK 1989-1685	19890407
DK 162521	B	19911111		
DK 162521	C	19920330		

PRIORITY APPLN. INFO.:	AU 1979-9617	19790717
	AU 1980-3093	19800411
	US 1980-164933	19800701
	EP 1980-302411	19800717
	AU 1981-7201	19810112
	US 1981-334384	19811224

GI



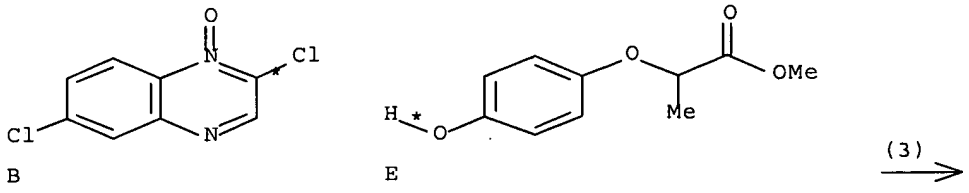
I



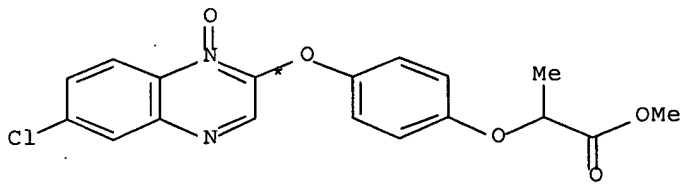
II

AB The title compds. I (X = optionally substituted OC6H4O, OC6H4S, SC6H4S; R = H, optionally substituted alkyl, acyl; R1 = H, optionally substituted alkyl; RR1 = alkylene; R2 = cyano, carbamoyl, optionally esterified CO2H, substituted Me; R3 = H, halogen, cyano, thiocyano, optionally substituted NH2, aliphatic, OH, SH, CO2H, or CONH2; m, n = 0, 1; p = 0-2) were prepared Thus, 2,6-dichloroquinoxaline was treated with 4-HOC6H4OCHMeCO2Me to give 70% II. At 1 kg/ha preemergence II gave 100% control of ryegrass and Japanese millet.

RX(3) OF 4 ...B + **E** ===> **F**



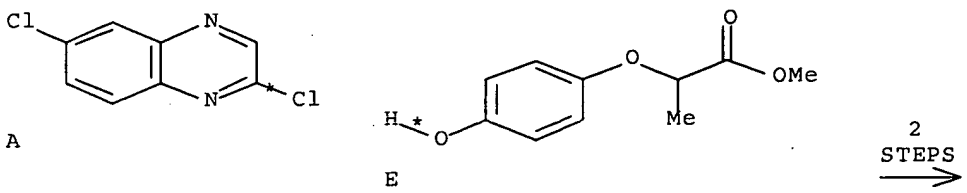
B E (3)



F

RX(3) RCT B 78104-57-1, E 60075-04-9
PRO F 78104-58-2

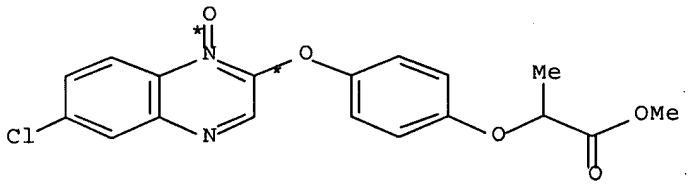
RX(4) OF 4 COMPOSED OF RX(1), RX(3)
RX(4) **A** + **E** ===> **F**



A

E

2 STEPS



F

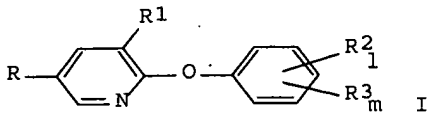
RX(1) RCT A 18671-97-1
PRO B 78104-57-1

RX(3) RCT B 78104-57-1, E **60075-04-9**
PRO F **78104-58-2**

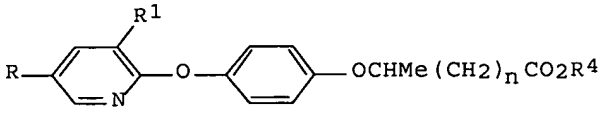
L48 ANSWER 18 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 94:103186 CASREACT Full-text
TITLE: 4-(2-Pyridyloxy)phenoxyalkanecarboxylic acids and their derivatives
PATENT ASSIGNEE(S): Ishihara Sangyo Kaisha, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55139361	A	19801031	JP 1979-48147	19790419
JP 63043389	B	19880830		
US 4267336	A	19810512	US 1980-137954	19800407
GB 2048864	A	19801217	GB 1980-12507	19800416
GB 2048864	B	19830525		
FR 2454439	A1	19801114	FR 1980-8831	19800418
FR 2454439	B1	19830624		
BR 8002431	A	19801202	BR 1980-2431	19800418

PRIORITY APPLN. INFO.: JP 1979-48147 19790419
GI



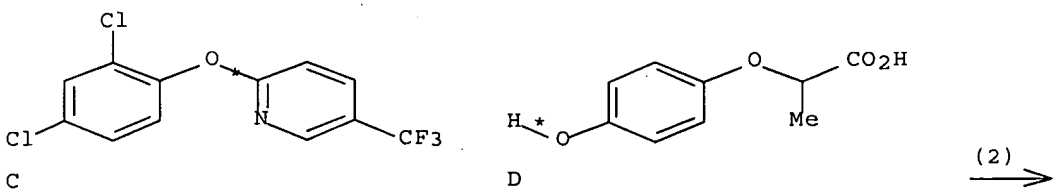
I



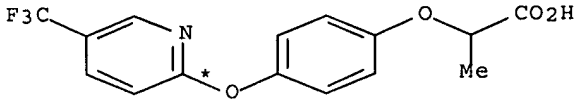
III

AB Phenoxypyridines I (R = halo, CF3; R1 = H, halo; R2 = Me; R3 = halo; l = 0-2; m = 0-5) were treated with p-HOC6H4OCHMe(CH2)nCO2R4 (II; R4 = H, alkyl, cation; n = 0, 2) or their derivs. to give III. Thus, heating 5.4 g 2-chloro-5-trifluoromethylpyridine with 2,6-Cl2C6H3OH and KOH in Me2SO 3 h at 110° gave 7.5 g corresponding I, which (2 g) was heated with II (R4 = H, n = 0) and KOH in Me2SO 4 h at 100° to give 1.3 g corresponding III.

RX(2) OF 3 ...C + D ===> E



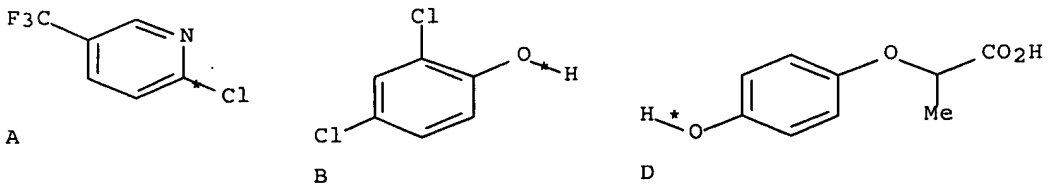
C D (2)



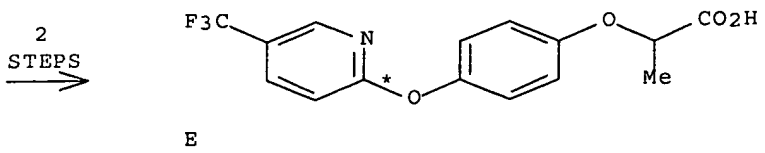
E

RX(2) RCT C 105626-83-3, D 67648-61-7
PRO E 69335-91-7

RX(3) OF 3 COMPOSED OF RX(1), RX(2)
RX(3) A + B + D ===> E



A B D



E

RX(1) RCT A 52334-81-3, B 120-83-2
PRO C 105626-83-3

RX(2) RCT C 105626-83-3, D 67648-61-7
PRO E 69335-91-7

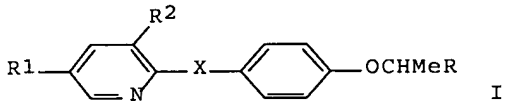
L48 ANSWER 19 OF 27 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 90:203882 CASREACT Full-text
TITLE: [[[(Trifluoromethyl)pyridyl]oxy]phenoxy]propionic acid and analogs
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54024879	A	19790224	JP 1978-89287	19780721
JP 63050345	B	19881007		
CA 1247625	A1	19881227	CA 1978-305900	19780621
EP 483	A1	19790207	EP 1978-100291	19780630
EP 483	B1	19811014		
R: BE, DE, FR, GB, NL, SE				
EP 57473	A2	19820811	EP 1982-101502	19780630
EP 57473	A3	19830511		
R: BE, DE, FR, GB, NL, SE				
AU 7837703	A	19800110	AU 1978-37703	19780703
AU 519094	B2	19811105		
DK 7803260	A	19790123	DK 1978-3260	19780721
DK 156830	B	19891009		
DK 156830	C	19900312		
BR 7804724	A	19790410	BR 1978-4724	19780721
BR 7804725	A	19790410	BR 1978-4725	19780721
AU 8063039	A	19810205	AU 1980-63039	19801007
AU 529649	B2	19830616		
JP 56123971	A	19810929	JP 1980-141111	19801008
JP 63044148	B	19880902		
EP 17767	A1	19801029	EP 1980-101361	19801029
EP 17767	B1	19830302		
R: BE, DE, FR, GB, NL, SE				
CA 1321590	C2	19930824	CA 1981-388668	19811023
JP 58083675	A	19830519	JP 1982-173144	19821001
JP 58090553	A	19830530	JP 1982-173143	19821001
JP 63052026	B	19881017		
JP 58099464	A	19830613	JP 1982-173142	19821001

US 4479001	A	19841023	US 1983-467552	19830217
JP 58201766	A	19831124	JP 1983-66813	19830415
JP 59062567	A	19840410	JP 1983-129293	19830715
JP 59062568	A	19840410	JP 1983-129296	19830715
JP 59067202	A	19840416	JP 1983-129292	19830715
JP 63013961	B	19880329		
JP 59067267	A	19840416	JP 1983-129294	19830715
JP 01003192	B	19890119		
JP 59067268	A	19840416	JP 1983-129295	19830715
JP 63044747	B	19880906		
JP 59130271	A	19840726	JP 1983-147929	19830812
US 4523017	A	19850611	US 1983-529178	19830902
US 4551170	A	19851105	US 1984-679976	19841210
JP 61106503	A	19860524	JP 1985-207714	19850919
JP 63017801	B	19880415		
JP 63152302	A	19880624	JP 1987-206201	19870819
JP 02019109	B	19900427		
PRIORITY APPLN. INFO.:			US 1977-817943	19770722
			CA 1978-305900	19780621
			US 1978-918550	19780623
			AU 1978-37703	19780703
			EP 1980-101361	19801029
			US 1982-357346	19820311
			US 1982-409791	19820820

OTHER SOURCE(S): MARPAT 90:203882

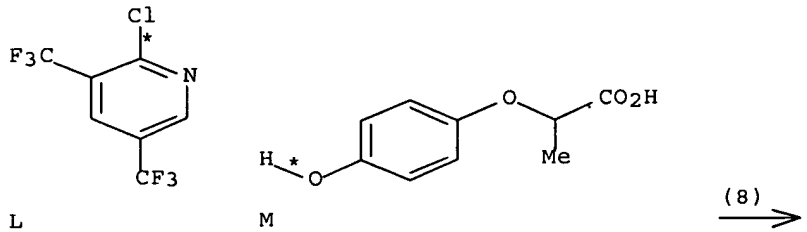
GI



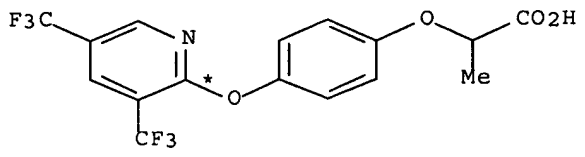
I

AB The title compds. [I, R = COR3 (R3 = OH, alkoxy, NH2, alkylamino), CN, CH2OH; R1, R2 = Cl, CF3; X = O, S] were prepared and their herbicidal activity evaluated. Thus, p-HOC6H4OCHMeCO2H in MeSO-NaOH-H2O was treated with 2-chloro-3,5-bis(trifluoromethyl)pyridine at 110° for 35 min to give I (R = CO2H, R1 = R2 = CF3, X = O).

RX(8) OF 36 L + M ===> N



L M



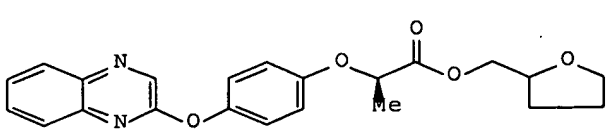
N

RX(8) RCT L 70158-60-0, M 67648-61-7
PRO N 70158-55-3

L48 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:571472 CAPLUS Full-text
DOCUMENT NUMBER: 117:171472
TITLE: optically active (R)-4-[[(2-quinoxalinyl)oxy]phenoxy]propionates and a process for their preparation
INVENTOR(S): Zeiss, Hans Joachim; Mildenberger, Hilmar
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 492629	A2	19920701	EP 1991-122231	19911224
EP 492629	A3	19930113		
EP 492629	B1	19950920		
R: BE, CH, DE, FR, GB, IT, LI, NL				
DE 4042098	A1	19920702	DE 1990-4042098	19901228
DE 4042098	C2	19931007		
BR 9105529	A	19920901	BR 1991-5529	19911219
ZA 9110055	A	19920930	ZA 1991-10055	19911220
CA 2058320	A1	19920629	CA 1991-2058320	19911223
AU 9190080	A	19920702	AU 1991-90080	19911224
AU 653376	B2	19940929		
JP 04295469	A	19921020	JP 1991-345246	19911226
IL 100531	A	19960331	IL 1991-100531	19911226
HU 61291	A2	19921228	HU 1991-4124	19911227
HU 208682	B	19931228		

PRIORITY APPLN. INFO.: DE 1990-4042098 A 19901228
OTHER SOURCE(S): CASREACT 117:171472; MARPAT 117:171472
ED Entered STN: 01 Nov 1992
GI



I

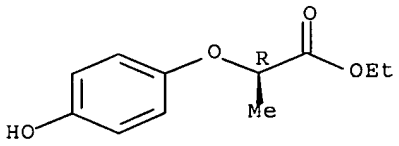
AB A process for the preparation of optically active C1-18-alkyl, benzyl, cycloalkyl, or alkenyl (R)-4-[[(2-quinoxalinyl)oxy]phenoxy]propionates comprises the condensation reaction of a 2-substituted quinoxaline with a lower alkyl (R)-2-(4-hydroxyphenoxy)propionate and transesterification of the ester thus obtained without racemization. The title compds. are herbicides, whereby the (R)-isomers have a greater biol. activity than the (S)-isomers (no data). A mixture of 2,6-dichloroquionoxaline (5.00 g), Et D-2-(4-hydroxyphenoxy)propionate (5.40 g), potassium carbonate (3.50 g), polyethylene glycol (0.3 g) and xylene was refluxed for 6 h to give Et (R)-2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]propionate in 91.1% yield (82% optically pure). Transesterification of the latter with (±)-tetrahydrofurfuryl alc. gave (±)-tetrahydrofurfuryl (R)-2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]propionate (I) in 88.6% yield.

IT 71301-98-9, Ethyl (R)-2-(4-hydroxyphenoxy)propionate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with dichloroquinoxaline)

RN 71301-98-9 CAPLUS

CN Propanoic acid, 2-(4-hydroxyphenoxy)-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

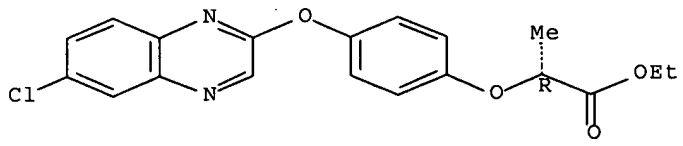


IT 100646-51-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and transesterification of)

RN 100646-51-3 CAPLUS

CN Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

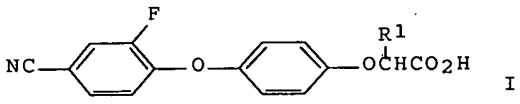


L48 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:552054 CAPLUS Full-text
DOCUMENT NUMBER: 113:152054
TITLE: Preparation of herbicidal [(cyanofluorophenoxy)phenoxy]alkanoic acids and derivatives
INVENTOR(S): Pews, R. Garth; Jackson, Lucinda A.; Carson, Chrislyn

M.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 17 pp. Cont.-in-part of U.S. Ser. No. 82,030, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4894085	A	19900116	US 1988-277619	19881129
ES 2045018	T3	19940116	ES 1988-109559	19880615
AU 8819061	A	19890209	AU 1988-19061	19880714
AU 605327	B2	19910110		
BR 8804034	A	19890228	BR 1988-4034	19880802
JP 01066156	A	19890313	JP 1988-195283	19880804
JP 06078293	B	19941005		
US 4980494	A	19901225	US 1989-448047	19891208
PRIORITY APPLN. INFO.:			US 1987-82030 B2	19870805
			US 1988-277619 A3	19881129

OTHER SOURCE(S): MARPAT 113:152054
ED Entered STN: 27 Oct 1990
GI



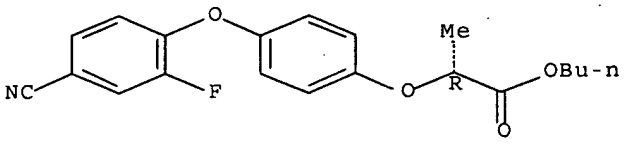
I

AB Title acids I (R1 = C1-3 alkyl) and their opticl isomers and agriculturally acceptable acid-group derivs. (esters, salts, amides, alcs., halides, tetrazoles, nitriles, etc.) are prepared as selective postemergent herbicides for grassy weeds, useful in wheat, barley, and especially rice. Thus, etherification of 4-HOC6H4OCHMeCO2Me with 3,4-F2C6H3CN using NaOH in DMSO at 80° gave I (R1 = Me) Me ester. This underwent saponification with KOH-MeOH, conversion to the acid chloride with SOCl2, and reesterification with BuOH-pyridine in CCl4 to give the Bu ester (II). In a postemergent paddy test, II at 200 g/ha gave 92% control of Leptochloa filiformis without damage to rice. Eighteen syntheses, 8 formulations, and numerous postemergent tests are described.

IT **122008-85-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

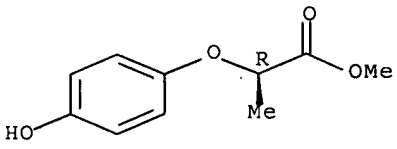
RN 122008-85-9 CAPLUS
CN Propanoic acid, 2-[4-(4-cyano-2-fluorophenoxy)phenoxy]-, butyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 96562-58-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of herbicides)
RN 96562-58-2 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L48 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:496861 CAPLUS Full-text
DOCUMENT NUMBER: 111:96861
TITLE: Herbicidal [(fluorocyanophenoxy)phenoxy]alkanoates, their compositions, use, and preparation
INVENTOR(S): Pews, Garth R.; Jackson, Lucinda A.; Carson, Chrislyn M.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: Eur. Pat. Appl., 25 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

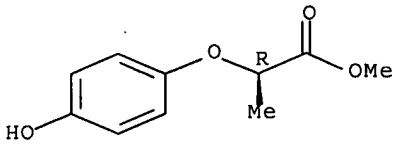
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 302203	A1	19890208	EP 1988-109559	19880615
EP 302203	B1	19921028		
R: BE, DE, ES, FR, GB, IT, NL				
ES 2045018	T3	19940116	ES 1988-109559	19880615
AU 8819061	A	19890209	AU 1988-19061	19880714
AU 605327	B2	19910110		
BR 8804034	A	19890228	BR 1988-4034	19880802
JP 01066156	A	19890313	JP 1988-195283	19880804
JP 06078293	B	19941005		
PRIORITY APPLN. INFO.:			US 1987-82030 A	19870805

OTHER SOURCE(S): MARPAT 111:96861
ED Entered STN: 16 Sep 1989
GI For diagram(s), see printed CA Issue.
AB Title acids I (R1 = C1-3 alkyl; R2 = H) and their enantiomers and/or derivs. are prepared as selective herbicides, especially for controlling grassy weeds in crops such as wheat, barley, and especially rice. Etherification of 4-

HOC6H4OCHMeCO2Me with 3,4-F2C6H3CN in Me2SO containing NaOH at 80° gave I (R1 = R2 = Me) (II). At 560 g/ha postemergence under paddy conditions, II completely killed Echinochloa crus-galli and Leptochloa filiformis without phytotoxicity to rice.

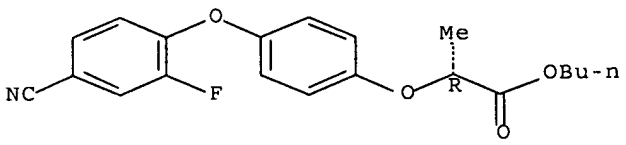
IT 96562-58-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of, with difluorobenzonitrile)
RN 96562-58-2 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 122008-85-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 122008-85-9 CAPLUS
CN Propanoic acid, 2-[4-(4-cyano-2-fluorophenoxy)phenoxy]-, butyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:204504 CAPLUS Full-text
DOCUMENT NUMBER: 108:204504
TITLE: Propynyl [(pyridinyloxy)phenoxy]propionate, a procedure for its preparation, and its use as a herbicide and grass growth inhibitor
INVENTOR(S): Schurter, Rolf
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 248968	A1	19871216	EP 1986-810300	19860707

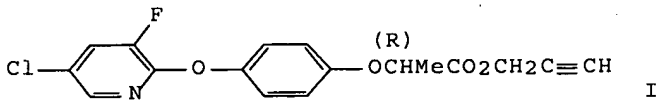
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE

CH 679396	A5	19920214	CH 1986-2376	19860612
DK 8603071	A	19871213	DK 1986-3071	19860627
DK 162216	B	19910930		
DK 162216	C	19920316		
FI 8602769	A	19871213	FI 1986-2769	19860630
FI 87772	B	19921113		
FI 87772	C	19930225		
NO 8602665	A	19871214	NO 1986-2665	19860701
NO 168528	B	19911125		
NO 168528	C	19920304		
AU 8659491	A	19871217	AU 1986-59491	19860702
AU 592804	B2	19900125		
DD 253754	A5	19880203	DD 1986-292079	19860702
DD 272069	A5	19890927	DD 1986-312694	19860702
ZA 8604947	A	19880224	ZA 1986-4947	19860703
CS 261243	B2	19890112	CS 1986-5038	19860703
IL 79330	A	19891215	IL 1986-79330	19860703
HU 41602	A2	19870528	HU 1986-2832	19860707
HU 206243	B	19921028		
CA 1236106	A1	19880503	CA 1986-513270	19860708
JP 62292758	A	19871219	JP 1986-165450	19860714
JP 05029221	B	19930428		
ES 2000663	A6	19880316	ES 1986-276	19860714
PL 147477	B1	19890630	PL 1986-260614	19860714
BR 8603381	A	19880209	BR 1986-3381	19860717
SU 1567116	A3	19900523	SU 1986-4027879	19860731
CN 86104887	A	19871223	CN 1986-104887	19860805
ES 2007331	A6	19890616	ES 1987-267	19870205

PRIORITY APPLN. INFO.: CH 1986-2376 A 19860612

ED Entered STN: 11 Jun 1988

GI



I

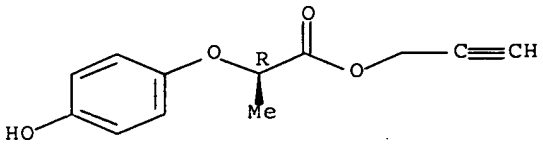
AB The title compound (I), useful as a herbicide and plant growth regulator (no data), was prepared by 6 methods. I was prepared in 4 steps from 2,5-dichloro-3-nitropyridine (II). Ten formulations were given, with ingredients as percentages.

IT **114365-33-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of, with chlorodifluoropyridine)

RN 114365-33-2 CAPLUS

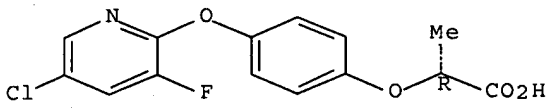
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, 2-propynyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 114420-56-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to acid chloride)
RN 114420-56-3 CAPLUS
CN Propanoic acid, 2-[4-[(5-chloro-3-fluoro-2-pyridinyl)oxy]phenoxy]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

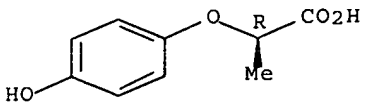


L48 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:625789 CAPLUS Full-text
DOCUMENT NUMBER: 105:225789
TITLE: Resolution of 2-(4-hydroxyphenoxy)propionic acid
INVENTOR(S): Matsumoto, Hiroo; Obara, Yoshio; Arai, Kazutaka; Tsuchiya, Shuji
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61083144	A	19860426	JP 1984-204363	19840928
JP 05017214	B	19930308		
PRIORITY APPLN. INFO.:			JP 1984-204363	19840928

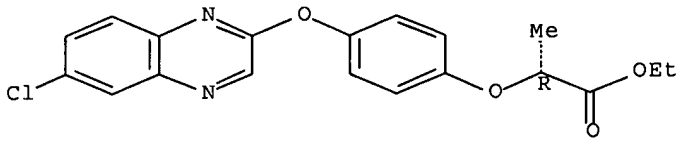
ED Entered STN: 26 Dec 1986
AB The title compound (I), useful as an intermediate for herbicides, was prepared by resolving racemic or partially-resolved I using optically-active RC6H4CH(NH2)CH2R1 (II; R = H, halo, alkyl, NO2; R1 = H, OH, alkyl). Thus, a solution of racemic I in EtOH was stirred with (-)-II (R = R1 = H) at 28-30° to give 47.5% diastereomeric salts, which were separated and decomposed. (+)-I of 100% enantiomeric excess was crystallized from EtOH. (-)-I could be obtained from the filtrate by repeating the process with (+)-II (R = R1 = H).
IT 94050-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 94050-90-5 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 100646-51-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for herbicides)
RN 100646-51-3 CAPLUS
CN Propanoic acid, 2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

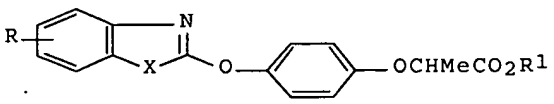


L48 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:455094 CAPLUS Full-text
DOCUMENT NUMBER: 101:55094
TITLE: Benzoxazolyl- and benzothiazolyloxyphenoxypropionic acid derivatives
INVENTOR(S): Zeiss, Hans Joachim; Mildenberger, Hilmar; Handte, Reinhardt
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

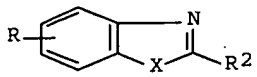
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3236730	A1	19840405	DE 1982-3236730	19821004
EP 105494	A2	19840418	EP 1983-109804	19830930
EP 105494	A3	19851106		
EP 105494	B1	19880810		
R: CH, DE, FR, GB, IT, LI, NL				
IL 69875	A	19870916	IL 1983-69875	19830930
BR 8305451	A	19840515	BR 1983-5451	19831003
JP 59084877	A	19840516	JP 1983-183237	19831003
JP 05001263	B	19930107		
ZA 8307379	A	19840627	ZA 1983-7379	19831003
HU 32576	A2	19840828	HU 1983-3436	19831003
HU 189752	B	19860728		
CA 1210403	A1	19860826	CA 1983-438222	19831003

PRIORITY APPLN. INFO.: DE 1982-3236730 A 19821004
OTHER SOURCE(S): CASREACT 101:55094; MARPAT 101:55094

ED Entered STN: 18 Aug 1984
GI



I



II

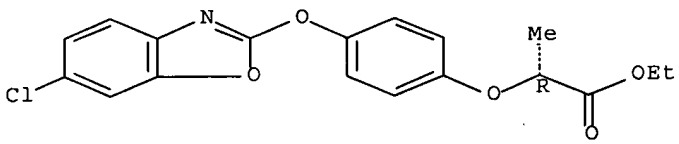
AB The title compds. I [X = O, S; R = halogen, CF3; R1 = (un)substituted alkyl] were prepared by treating halobenzazoles II (R2 = halogen) with 4-HOC6H4OCHMeCO2R1 in presence of quaternary ammonium or phosphonium or a polyalkylene glycol catalyst. Thus 2,6-dichlorobenzothiazole was treated with 4-HOC6H4OCHMeCO2Et in the presence of Bu4P+Br- to give 96.8% I (X = S, R = 6-Cl, R1 = Et) of >97% purity.

IT **71283-80-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 71283-80-2 CAPLUS

CN Propanoic acid, 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

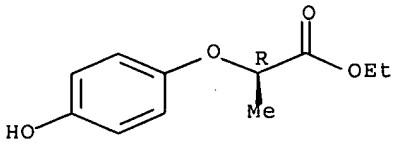


IT 71301-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with halobenzazoles)

RN 71301-98-9 CAPLUS

CN Propanoic acid, 2-(4-hydroxyphenoxy)-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

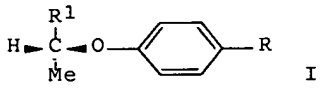


L48 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:424528 CAPLUS Full-text
DOCUMENT NUMBER: 95:24528
TITLE: Optically active α-phenoxypropionic acid derivatives for herbicides
INVENTOR(S): Nestler, Hans Juergen; Hoerlein, Gerhard; Handte,

Reinhard; Bieringer, Hermann; Schwerdtle, Friedhelm; Langelueddeke, Peter; Frisch, Peter
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Brit. UK Pat. Appl., 21 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2042503	A	19800924	GB 1979-2307	19790122

PRIORITY APPLN. INFO.: GB 1979-2307 A 19790122
ED Entered STN: 12 May 1984
GI



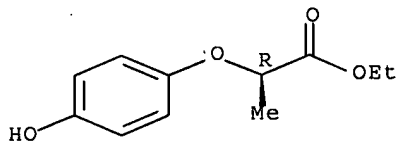
I

AB The title compds. I [R = optionally substituted (o.s.) PhO, o.s. 2-pyridyloxy, o.s. 2-benzoxazolyloxy, o.s. 2-benzothiazolyloxy, o.s. CH2Ph; R1 = o.s. CO2H, o.s. C(O)SH, o.s. CONH2, o.s. CONHNH2, o.s. CSNH2] were prepared E.g., 4-ClC6H4OC6H4OH-4 condensed with L-lactic acid Et ester toluenesulfonate in the presence of K2CO3 (MeCOEt, reflux, 56 h) to give 97% I (R = OC6H4Cl-4, R1 = CO2Et). I are more potent herbicides than their racemic analogs, e.g. the ED (ED95) of I (R = OC6H4Cl-4, R1 = CO2CH2CHMe2) in the postemergence treatment of annual blackgrass in sugar beet was 0.44 kg/ha whereas that of the racemic analog was 0.76 kg/ha.

IT **71301-98-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with dichlorobenzoxazole or nitrochlorobenzotrifluoride)

RN 71301-98-9 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

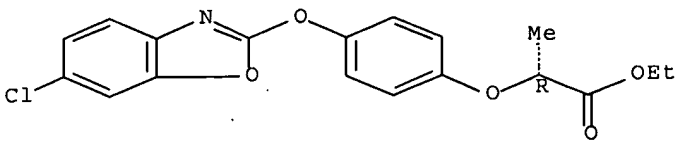


IT **71283-80-2P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

RN 71283-80-2 CAPLUS
CN Propanoic acid, 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-, ethyl ester,

(2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

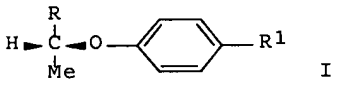


L48 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:540579 CAPLUS Full-text
DOCUMENT NUMBER: 91:140579
TITLE: Optically-active aryloxypropionic acid derivatives for use as herbicides
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Belg., 50 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 873844	A1	19790516	BE 1979-193191	19790131
DE 2758002	A1	19790705	DE 1977-2758002	19771224
ES 476100	A1	19790416	ES 1978-476100	19781218
EP 2800	A1	19790711	EP 1978-101792	19781220
EP 2800	B1	19811202		
EP 2800	B2	19911009		
R: BE, DE, FR, GB, IT, NL, SE				
US 4531969	A	19850730	US 1978-971427	19781220
ZA 7807210	A	19791227	ZA 1978-7210	19781221
DK 7805790	A	19790625	DK 1978-5790	19781222
DK 156511	B	19890904		
DK 156511	C	19950522		
AU 7842849	A	19790628	AU 1978-42849	19781222
AU 527127	B2	19830217		
BR 7808443	A	19790821	BR 1978-8443	19781222
DD 141403	A5	19800430	DD 1978-210128	19781222
RO 75478	A1	19810330	RO 1978-96022	19781222
CS 204959	B2	19810430	CS 1978-8850	19781222
AT 7809212	A	19820215	AT 1978-9212	19781222
AT 368357	B	19821011		
RO 79065	A1	19820625	RO 1978-99034	19781222
HU 25775	A2	19830829	HU 1978-HO2126	19781222
HU 182883	B	19840328		
SU 1336939	A3	19870907	SU 1978-2700051	19781222
IL 56283	A	19870916	IL 1978-56283	19781222
CA 1268475	A1	19900501	CA 1978-318525	19781222
JP 54112828	A	19790904	JP 1978-158179	19781223
PL 122180	B1	19820630	PL 1978-212111	19781223
FR 2447366	A1	19800822	FR 1979-1604	19790123
FR 2447366	B1	19841116		
SU 1075969	A3	19840223	SU 1981-3233698	19810120
JP 63211250	A	19880902	JP 1987-251741	19871007

US 5254527	A	19931019	US 1991-790128		19911107
US 5712226	A	19980127	US 1995-465889		19950606
PRIORITY APPLN. INFO.:			DE 1977-2758002	A	19771224
			FR 1979-1604		19790123
			US 1978-971427	A3	19781220
			US 1985-730295	B1	19850503
			US 1988-144612	B1	19880111
			US 1989-434490	B1	19891109
			US 1991-663274	B1	19910228
			US 1991-790128	A3	19911107
			US 1993-98452	B1	19930727
			US 1994-238974	B1	19940505
			US 1995-400175	B1	19950306

OTHER SOURCE(S): MARPAT 91:140579
ED Entered STN: 12 May 1984
GI

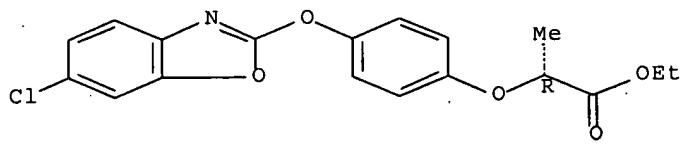


I

AB 2-Phenoxypropionic acid derivs. I [R = CO2R2 [R2 = H, alkyl, cycloalkyl, halocycloalkyl, cycloalkenyl, alkynyl, or alkyl-, alkoxy-, halo-, nitro-, or (trifluoromethyl)phenyl], C(O)SR3 (R3 = alkyl, alkenyl, alkylphenyl, halophenyl), CONR4R5 [R4 and R5 are independently H, alkyl, hydroxyalkyl, cycloalkyl, or alkyl-, alkoxy-, halo-, or (trifluoromethyl)phenyl], CONR6NR7R8 (R6 = H, Me; R7 = H, Me, Et; R8 = H, Me, Et, Ph), CSNH2; R1 = 2-phenoxy, 2-pyridyloxy, benzoxazol-2-yloxy, benzothiazol-2-yloxy, or benzyl group], which showed herbicidal activity, were prepared from lactate esters and phenols. 4-(4-Chlorophenoxy)phenol, Et L-(-)-O-tosyllactate, and K2CO3 in MeCOEt were refluxed 56 h to yield I (R = CO2Et, R1 = 4-ClC6H4O).

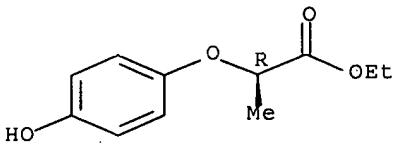
IT 71283-80-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 71283-80-2 CAPLUS
CN Propanoic acid, 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 71301-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(O-arylation of)
RN 71301-98-9 CAPLUS
CN Propanoic acid, 2-(4-hydroxyphenoxy)-, ethyl ester, (2R)- (9CI) (CA INDEX NAME)

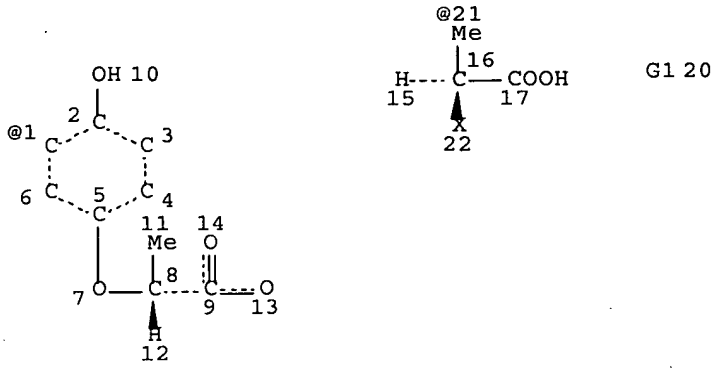
Absolute stereochemistry. Rotation (+).



FILE 'HOME' ENTERED AT 10:51:23 ON 18 DEC 2006

SEARCH HISTORY

=> d stat que l24; d stat que l31; d stat que l25; d stat que l36; d his nofile
L17 STR



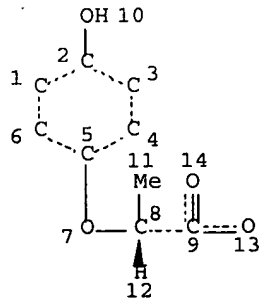
VAR G1=1/21
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 2

L19	72	SEA FILE=REGISTRY SSS FUL L17
L20	49	SEA FILE=REGISTRY ABB=ON 46.150.18/RID AND L19
L21	23	SEA FILE=REGISTRY ABB=ON L19 NOT L20
L22	412	SEA FILE=CAPLUS ABB=ON L21
L23	115	SEA FILE=CAPLUS ABB=ON L20
L24	15	SEA FILE=CAPLUS ABB=ON L22 AND L23

L26 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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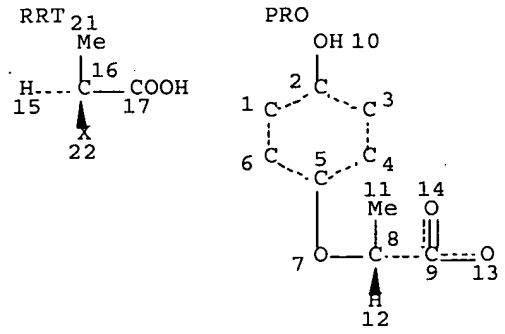
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1
L28           97 SEA FILE=CASREACT SSS FUL L26 (    747 REACTIONS)
L29              STR
```

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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

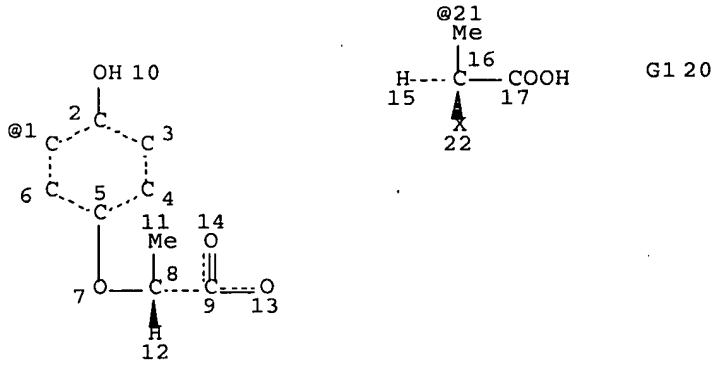
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  19

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 2
L31            5 SEA FILE=CASREACT SUB=L28 SSS FUL L29 (     18 REACTIONS)

100.0% DONE      28 VERIFIED      18 HIT RXNS                          5 DOCS
SEARCH TIME: 00.00.01



L3             1 SEA FILE=REGISTRY ABB=ON  72619-32-0
L4             1 SEA FILE=REGISTRY ABB=ON  114420-56-3
L6             1 SEA FILE=REGISTRY ABB=ON  FLUAZIFOP-P-BUTYL/CN
L10            1 SEA FILE=REGISTRY ABB=ON  CYHALOFOP-BUTYL/CN
L11            1 SEA FILE=REGISTRY ABB=ON  QUIZALOFOP-P-ETHYL/CN
L12            1 SEA FILE=REGISTRY ABB=ON  71283-80-2
L13            6 SEA FILE=REGISTRY ABB=ON  (L11 OR L3 OR L6 OR L4 OR L10 OR
                 L12)
L14           28 SEA FILE=CAPLUS ABB=ON  L13/P
L17              STR
```

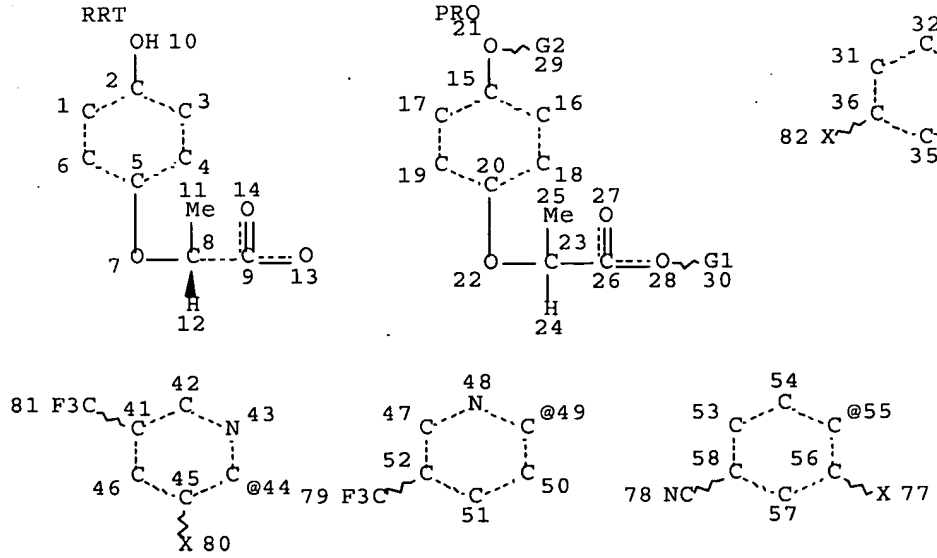


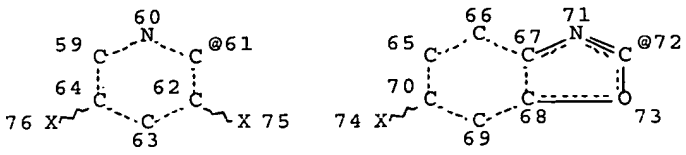
VAR G1=1/21
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 2
L19 72 SEA FILE=REGISTRY SSS FUL L17
L20 49 SEA FILE=REGISTRY ABB=ON 46.150.18/RID AND L19
L23 115 SEA FILE=CAPLUS ABB=ON L20
L25 11 SEA FILE=CAPLUS ABB=ON L23 AND L14

L34 STR





Page 2-A
VAR G1=H/ME/ET/N-BU
VAR G2=38/44/49/55/61/72
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 82

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1
L36 19 SEA FILE=CASREACT SSS FUL L34 (70 REACTIONS)

100.0% DONE 424 VERIFIED 70 HIT RXNS 19 DOCS
SEARCH TIME: 00.00.01

(FILE 'HOME' ENTERED AT 09:20:42 ON 18 DEC 2006)

FILE 'CAPLUS' ENTERED AT 09:21:05 ON 18 DEC 2006
E US2006-571863/APPS
L1 1 SEA ABB=ON US2006-571863/AP
D SCAN
SEL RN

FILE 'REGISTRY' ENTERED AT 09:21:37 ON 18 DEC 2006
L2 19 SEA ABB=ON (14265-45-3/BI OR 15181-46-1/BI OR 100646-51-3/BI OR 114420-56-3/BI OR 122008-85-9/BI OR 123-31-9/BI OR 14844-07-6/BI OR 23134-05-6/BI OR 29617-66-1/BI OR 302-01-2/BI OR 50-81-7/BI OR 62607-44-7/BI OR 71283-80-2/BI OR 72619-32-0/BI OR 7446-09-5/BI OR 74533-11-2/BI OR 7631-90-5/BI OR 79241-46-6/BI OR 94050-90-5/BI)
D SCAN

FILE 'CAPLUS' ENTERED AT 09:27:05 ON 18 DEC 2006
D SCAN L1

FILE 'REGISTRY' ENTERED AT 09:27:06 ON 18 DEC 2006
L3 1 SEA ABB=ON 72619-32-0
D SCAN
L4 1 SEA ABB=ON 114420-56-3
D SCAN
E HALOXYFOP-P-METHYL/CN
L5 1 SEA ABB=ON HALOXYFOP-P-METHYL/CN
D SCAN
E FLUAZIFOP-P-BUTYL/CN

```
L6            1 SEA ABB=ON  FLUAZIFOP-P-BUTYL/CN
                D SCAN
                E FENOXAPROP-P-ETHYL/CN
L7            1 SEA ABB=ON  "FENOXAPROP-P-ETHYL-BENSULFURON METHYL MIXT."/CN
                D SCAN
L8              STR

     FILE 'CAPLUS' ENTERED AT 10:12:25 ON 18 DEC 2006
                D SCAN L1

     FILE 'REGISTRY' ENTERED AT 10:12:26 ON 18 DEC 2006
L9            1 SEA ABB=ON  L3 OR L5
                E CYHALOFOP-BUTYL/CN
L10           1 SEA ABB=ON  CYHALOFOP-BUTYL/CN
                D SCAN
                E QUIZALOFOP-P-ETHYL/CN
L11           1 SEA ABB=ON  QUIZALOFOP-P-ETHYL/CN
                D SCAN
                D SCAN L7
                D IDE L7
L12           1 SEA ABB=ON  71283-80-2
                D SCAN
L13           6 SEA ABB=ON  (L11 OR L3 OR L6 OR L4 OR L10 OR L12)

     FILE 'CAPLUS' ENTERED AT 10:18:07 ON 18 DEC 2006
L14          28 SEA ABB=ON  L13/P

     FILE 'REGISTRY' ENTERED AT 10:19:19 ON 18 DEC 2006
L15             STR L8
L16           9 SEA SSS SAM L15
L17             STR L15
L18           6 SEA SSS SAM L17
                D SCAN
L19          72 SEA SSS FUL L17
                SAVE TEMP L19 NAG863FULL/A
L20          49 SEA ABB=ON  46.150.18/RID AND L19
                SAVE TEMP L20 NAG863SUB1/A
L21          23 SEA ABB=ON  L19 NOT L20
                SAVE TEMP L21 NAG863SUB2/A

     FILE 'CAPLUS' ENTERED AT 10:28:00 ON 18 DEC 2006
L22         412 SEA ABB=ON  L21
L23         115 SEA ABB=ON  L20
L24          15 SEA ABB=ON  L22 AND L23
L25          11 SEA ABB=ON  L23 AND L14
                D SCAN TI L25

     FILE 'CASREACT' ENTERED AT 10:30:03 ON 18 DEC 2006
L26             STR L17
L27           8 SEA SSS SAM L26 (   210 REACTIONS)
L28          97 SEA SSS FUL L26 (   747 REACTIONS)
                SAVE TEMP L28 NAG863CASRF/A
L29             STR L17
L30           1 SEA SUB=L28 SSS SAM L29 (    13 REACTIONS)
                D SCAN
                D STAT QUE
L31           5 SEA SUB=L28 SSS FUL L29 (    18 REACTIONS)
                SAVE TEMP L31 NAG863CASRSB1/A NAG863CSRSB1/A
                D QUE L24
L32             STR L26
```

```
L33           2 SEA SUB=L28 SSS SAM L32 (     4 REACTIONS)
                D SCAN
L34             STR L32
L35           2 SEA SSS SAM L34 (     4 REACTIONS)
L36          19 SEA SSS FUL L34 (    70 REACTIONS)
                SAVE TEMP L36 NAG863CSRSB2/A
                E CLEUGH/AU
L37           1 SEA ABB=ON  "CLEUGH ERNEST STEPHEN"/AU

     FILE 'CAPLUS' ENTERED AT 10:44:26 ON 18 DEC 2006
                E CLEUGH E/AU
L38           2 SEA ABB=ON  CLEUGH E?/AU
L39           1 SEA ABB=ON  L1 AND L38

     FILE 'CAPLUS' ENTERED AT 10:45:16 ON 18 DEC 2006
                D QUE NOS L38
L40           2 SEA ABB=ON  L38 OR (L38 AND (L24 OR L25))

     FILE 'CASREACT' ENTERED AT 10:45:37 ON 18 DEC 2006
                D QUE NOS L37
L41           1 SEA ABB=ON  L37 OR (L37 AND (L31 OR L36))

     FILE 'CASREACT, CAPLUS' ENTERED AT 10:45:56 ON 18 DEC 2006
L42           2 DUP REM L41 L40 (1 DUPLICATE REMOVED)
                      ANSWER '1' FROM FILE CASREACT
                      ANSWER '2' FROM FILE CAPLUS
                D IBIB ABS HIT 1
                D IBIB ED ABS HITSTR 2

     FILE 'CAPLUS' ENTERED AT 10:46:54 ON 18 DEC 2006
                D QUE L24
L43          14 SEA ABB=ON  L24 NOT L40

     FILE 'CASREACT' ENTERED AT 10:47:13 ON 18 DEC 2006
                D STAT QUE L31
L44           4 SEA ABB=ON  L31 NOT L41

     FILE 'CASREACT, CAPLUS' ENTERED AT 10:47:27 ON 18 DEC 2006
L45          16 DUP REM L44 L43 (2 DUPLICATES REMOVED)
                      ANSWERS '1-4' FROM FILE CASREACT
                      ANSWERS '5-16' FROM FILE CAPLUS
                D IBIB ABS HIT 1-4
                D IBIB ED ABS HITSTR 5-16

     FILE 'CAPLUS' ENTERED AT 10:48:37 ON 18 DEC 2006
                D QUE L25
L46          10 SEA ABB=ON  L25 NOT (L43 OR L40)

     FILE 'CASREACT' ENTERED AT 10:48:57 ON 18 DEC 2006
                D STAT QUE L36
L47          19 SEA ABB=ON  L36 NOT (L44 OR L41)

     FILE 'CASREACT, CAPLUS' ENTERED AT 10:49:28 ON 18 DEC 2006
L48          27 DUP REM L47 L46 (2 DUPLICATES REMOVED)
                      ANSWERS '1-19' FROM FILE CASREACT
                      ANSWERS '20-27' FROM FILE CAPLUS
                D IBIB ABS HIT 1-19
                D IBIB ED ABS HITSTR 20-27

     FILE 'HOME' ENTERED AT 10:51:23 ON 18 DEC 2006
```